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The Classification and Interpretation of the Amphiboles.

By

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ABSTRACT

This thesis reports a study of 2650 published chemical analyses of members of the amphibole group of minerals with a view to deriving a satisfactory nomenclature for the amphiboles, to outline the overall chemical variation exhibited by the group and the relation between amphibole composition and mode of occurrence.

To achieve these aims a computer program was developed to calculate atomic formulae and simplified or 'basic atomic formulae' from chemical analyses using an allocation scheme of cations between groups of sites derived from published experimentally determined cation distributions. The concept of the basic atomic formula was also used to make estimates of the iron oxidation state in electron microprobe analyses of amphiboles.

A large computer data base using a relational model of data is described and the value of such a data base strategy for the Geological Sciences is briefly discussed.

In order to achieve a simple and rational nomenclature an amended and extended version of 'amphibole compositional space' was devised in which calcic ($Na^X \leqslant 0.66$, $Mg^X \leqslant 0.66$), soda calcic (Na^X 0.66 - 1.33, $Mg^X \leqslant 0.66$) alkali ($Na^X > 1.33$) amphiboles were named according to the dominant component of their basic atomic formulae. Natural amphiboles close to miyashiroite and sundiusite were located and the validity of both previously discredited names discussed. An extended compositional space was devised to indicate the relation between calcic, soda calcic, alkali and FeMgMn ($Mg^X \geqslant 1.33$) amphiboles.

From the observed distribution of basic atomic formulae in amphibole compositional space and extended compositional space the importance of coupled isomorphous substitutions within the amphibole

structure and the extent of solvi within the amphibole group was considered. When the mode of occurrence was considered a number of interesting aspects of the complex relationship between amphibole composition and mode of occurrence became apparent.

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SYMBOLS AND ABBREVIATIONS

Site nomenclature.

A , M1 , M2 , M3 , M4 , T1 , T2 ,

O1, O2 , O3 , O4 , O5 , O6 , O7 .

Group nomenclature.

A group = A site,

X group = two M4 sites,

Y group = two M1, two M2, one M3 sites,

Z group = four T1, four T2 sites,

OH group = two O3 sites.

Ions

Fe^{3+} ion and oxidation state,

Al^{vi} ion and co-ordination number,

$\sum Y$ sum of the ions normally present in the Y group.

$\square$ vacancy,

Recalculation bases.

23(O) anion base of 23 oxygens

24(O) anion base of 24 oxygens

$\sum Na = 16$ cation base of 16 cations, A site full

$\sum Na = 15$ cation base of 15 cations, A site vacant

$\sum Ca = 15$ all cations except Na^+, K^+ normalised to 15

$\sum FM = 13$ all cations normally present in the Y and Z groups normalised to 13.

Basic atomic formula

$$Na^{A}, Ca, Na^{X*}, Mg, Al^{Y*}, Si\ Al^{Z*} O_{22} (OH)_2$$

Extended basic atomic formula

$$Na^{A}, Ca^{X*}, Mg^{X*}, Na^{X*}, Mg^{Y*}, Al^{Y*} Si\ Al^{Z*} O_{22} (OH)_2$$

* During typing X, Y and Z have occasionally been shown in lower case.

Additional basic atomic formulae components.

$Fe^{3+'}$ ferric iron component of Al^{Y},

$Al^{Y'}$ Al^{Y} excluding Fe^{3+}, $\therefore$ $Al^{Y} = Al^{Y'} + Fe^{3+'}$

$Al^{Y^{O}}$ Change in $Al^{Y'}$ with change in iron oxidation ratio.

1. INTRODUCTION

The amphiboles are an important group of hydrous monoclinic and orthorhombic chain silicates. The name amphibole was first proposed by Hauy in 1801 from the Greek amphibolos meaning ambiguous, in allusion to the then ambiguous nature of the mineral group. Following the first X-ray structure investigations of the monoclinic amphibole tremolite (Warren 1929) and the orthorhombic amphibole anthophyllite (Warren & Modell 1930) the general structural formula of the amphiboles was shown to be

$$A_{0-1}\ A_2\ Y_5\ Z_8\ O_{22}\ (OH)_2\ .$$

Typical ionic species in each group of sites are as follows:

Group	Typical ionic species
A	Na^+, K^+
X	Na^+, Ca^{2+}, Mn^{2+}, Fe^{2+}, Mg^{2+}, Li^+
Y	Mg^{2+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Ti^{4+}, Mn^{2+}, Cr^{3+}, Li^+
Z	Si^{4+}, Al^{3+}
OH	OH^-, F^-, Cl^-, O^{2-}

The reader unfamiliar with the structure and site nomenclature of the amphiboles is referred to Appendix 1 or to the excellent modern descriptions of specific crystal structures by Papike, Ross & Clark (1969), Papike & Ross (1970) and Hawthorne & Grundy (1973 a,b).

Amphiboles are found in a wide range of geological environments including contact and regionally metamorphosed rocks, igneous rocks of diverse character, and less commonly as an authigenic mineral in sedimentary rocks. In addition, amphiboles have been reported from meteorites (Olsen 1967; Douglas & Plant 1968; Olsen et al.

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1973), the moon (Agrell et al. 1970), and have been suggested as a possible phase in the Earth's mantle (Ringwood 1964; Mason 1968a). The compositional variation exhibited by the amphiboles is very great. Most of the major and many of the minor elements of the Earth's crust can enter the amphibole structure and because of this the group has been variously described as "wastebasket" (Ernst 1968) or "carpet bag" minerals (Gunn 1972). These features of widespread occurrence and variable composition make the amphiboles potentially very important in the interpretation of the physical and chemical conditions of formation of the rocks in which they occur. However, even though Leake in 1968 estimated that several thousand amphiboles had been analysed chemically, no clear understanding of their overall chemical variation and its relationship to mode of occurrence has emerged.

The chemical complexity of the amphiboles is reflected in their nomenclature. Felix (1970) catalogued over 300 names which had been proposed for varieties of amphibole. Add to this the difficulty in deriving an atomic formula due to the presence of water in the structure, the frequently incomplete nature of the chemical analyses, and the possibility of variations in order - disorder with temperature of crystallisation (Ghose & Weidner 1972; Seifert & Virgo 1974) and it can be seen that the amphiboles, even today, live up to their name. It is the aim of this work to propose aids to the interpretation and classification of chemical data relevant to the amphiboles and to use these and a large collection of published chemical analyses, to outline the overall chemical variation of the group and the relation between amphibole composition and mode of occurrence.

As a prerequisite to this it is desirable to be able to recast the weight per cent of the constituent oxides in a chemical

analysis into the relative numbers of ions present and to distribute these between the available crystallographic sites, or groups of sites in the structure. The derivation of an atomic formula from a chemical analysis is complicated in the amphiboles for the following three reasons:

(1) Chemical analyses are frequently incomplete. This applies in particular to determinations of H_2O+, F, Cl and the oxidation state of multivalent cations, in particular iron.

(2) The lack of a truly satisfactory anion or cation base from which the numbers of cations and anions present may be calculated. When accurate values for the density and cell volume of a specimen are known, an atomic formula can be calculated without recourse to an assumption concerning the number of cations or anions present (Hey 1939, 1954). However, this additional data is only rarely available and accurate values for the density are difficult to achieve.

(3) The allocation of ions to the crystallographic sites, or groups of sites, requires a knowledge of the distribution of ions in investigated specimens and how this is affected by bulk chemistry, and external conditions during crystallisation.

Considering the first two points together. Provided water and fluorine have been determined accurately a chemical analysis of an amphibole can be recalculated assuming an anion base of twenty four oxygens, 24(O), (O_{22}+ (O^{2-},OH^-,F^-)2). Errors in the value for H_2O+ or F will affect the resulting proportions of all cations. Miyashiro (1957) suggested that when H_2O+ and F were absent or inaccurately determined a hydroxyl free anion base of twenty three oxygens 23(O), (O_{22} + $\frac{1}{2}$ $(OH)_2 \equiv H_2O$) was to be preferred. When using the 23(O) base it is tactily assumed that the sum of hydroxyl and fluorine is two. Erroneous atomic formulae result if a 23(O)

base is applied to analyses of oxyamphiboles in which H^+ is deficient in the hydroxyl group, or to those in which protons enter the A site (Phillips 1963; Witte et al. 1969). With the advent of the widespread use of the electron microprobe, the number of analyses without water determined has increased and with it the use of the 23(O) anion base.

Borneman - Starÿnkevich (1960) suggested certain cation sums as alternatives to anion bases viz. Y + Z = 13, X + Y + Z = 15, $Si^{4+} + Al^{3+} = 8$ and $Si^{4+} = 6$. Other cation bases are plausible for example A + X + Y + Z = 16, Y = 5 but there is little justification for the general applicability of any of these (Phillips 1963). However, as described below cation bases have been employed in order to estimate the iron oxidation state in electron microprobe analyses (Stout 1972; Brady 1974).

In the last decade a considerable number of complete and partial site populations have been published for a variety of amphibole compositions (see Appendices 2 and 3). These have been determined by X-ray diffraction, infrared and Mössbauer spectroscopy. Starting from known site populations Whittaker (1960), Phillips (1963) and Ghose (1965) developed schemes whereby ions are allocated to the most appropriate site, or group of sites, in the crystal structure. Further, one of these schemes has been incorporated in an unpublished computer program entitled MINDATA3 (R. Phillips 1965 pers. comm.).

The writer evaluated Phillips' scheme by comparing published experimentally determined site populations with the site populations calculated for the same specimen from its chemical analysis alone. The scheme was found not to be entirely satisfactory. Starting from

published site populations a general scheme for allocation of ions between groups of sites (A = A, X = two M4, Y = two M2, two M1, M3, Z = four T1, four T2, OH = two O3) was devised, see Chapter 2, and incorporated into a computer program entitled MINDATA5.

Failure to determine the oxidation state of multivalent ions is most important with respect to iron, which is both ubiquitous and quantitatively important. With the advent of the widespread use of the electron microprobe in the analysis of amphiboles there exists a need for a satisfactory method whereby estimates of the iron oxidation state can be made. A semi-quantitative estimate has been made by analysis of the relative intensities of the $L\alpha$ and $L\beta$ emission lines (Albee & Chodos 1970).

There exist in addition a number of methods by which estimates of the iron oxidation state may be made given the total iron content and making certain assumptions as regards the crystal chemistry of the amphiboles. It should be noted that for most analyses in which the iron oxidation state has not been determined, water and fluorine are absent also. Starting with what may be called stoichiometric methods; these assume a cation base from which an atomic formula for the chemical analysis (all iron taken as FeO) may be calculated, see above. The sum of the number of oxygens associated with the cations is normally less than 23, the deficiency being taken as a measure of the Fe_2O_3 contribution.

Stout (1972) suggested four such cation bases. These were, (i) 16 cations, A site full, (ii) 15 cations, A site vacant, (iii) cations normally present in the Y and Z sites total 13 and (iv) cations normally present in the X, Y and Z groups total 15 excluding all Na^+ (and presumably all K^+ also). Stout favoured the fourth of these bases. Brady (1974) has followed a similar approach. Any

recalculation in terms of a cation base assumes that (i) all the remaining cations are determined accurately, (ii) the cation base is meaningful, see above,(iii) there are no anion vacancies other than those associated with undetermined Fe_2O_3 and (iv) that the amphibole is not an oxyamphibole. It can be shown that these assumptions do not hold in general. The choice of the recalculation base used depends a priori on a knowledge of the approximate composition of the amphibole under consideration. Thus, for example, the appropriate cation bases of Stout (1974) for a number of simple atomic formulae are set out below.

	appropriate cation base.
tremolite $\square Ca_2^{2+} Mg_5^{2+} Si_8^{4+}O_{22}^{2-} (OH^-)_2$	(ii,iii,iv)
richterite $Na^+ Ca^{2+} Na^+ Mg_5^{2+} Si_8^{4+}O_{22}^{2-} (OH^-)_2$	(i,iii)
cummingtonite $\square Mg_2^{2+} Mg_5^{2+} Si_8^{4+}O_{22}^{2-} (OH^-)_2$	(ii,iv)

Further, Phillips (1963) has suggested that Y group vacancies of the type $Ti^{4+} + \square = 2Mg^{2+}$, or less commonly $2R^{3+} + \square = 3R^{2+}$, may occur in the amphiboles. In practice stoichiometric methods often lead to oxygen totals in excess of 23.

Secondly in what Stout (1972) called chemical methods, an anion base of 23(O) is assumed. Atomic formulae are calculated with all the iron alternatively in the ferrous state (maximum number of cations) and the ferric state (minimum number of cations). The correct atomic formula is bracketed somewhere between these extremes. It may prove possible to apply certain constraints based on amphibole crystal chemical considerations (e.g. $Si^{4+} \leqslant 8.08$ atoms) to delimit the most likely oxidation state. However, as in the stoichiometric method, a number of assumptions must be made, (i) all the remaining ions are determined accurately, (ii) there are no oxygen vacancies

associated with the anion base and (iii) the specimen is not an oxyamphibole. Cation vacancies are permitted however.

One further possibility of determining the iron oxidation state is provided by the 'basic atomic formula' (Phillips & Layton 1964; Phillips 1966). The basic atomic formula was developed as an aid to the classification of the calciferous and alkali amphiboles (with Ca^{2+}, Na^{+} occupying the X group). The derivation is considered in greater detail below. To maintain charge balance in an accurate analysis the sum of basic atomic formula $Na^{A} + Al^{y}$ equals $Na^{X} + Al^{Z}$. As Fe^{3+} is included in Al^{y} but Fe^{2+} is not directly included in either Na^{A}, Al^{y}, Na^{X} or Al^{Z} (but see Chapter 3), calculation of basic atomic formulae for various iron oxidation states (total iron constant) might be expected to indicate only limited values for which the condition holds, and hence provide a useful estimate of the iron oxidation state in the analysis. The method was first suggested by Risch & Varnsars (1969) but as far as the author is aware has never been implemented. In Chapter 3 this method has been evaluated, initially for simple theoretical compositions with known oxidation states and then for genuine analyses.

Brief mention has already been made concerning the nomenclatural difficulties associated with the classification of the amphiboles. Minerals are normally classified in terms of chemical composition and crystal structure but amphibole varieties based on optical and physical properties or the mode of occurrence are still in vogue. Thus for example actinolite has been used for green amphiboles with atomic formulae approaching $\square Ca^{2+}_{2}(Mg^{2+}, Fe^{2+})_{5}Si^{4+}_{8}O^{2-}_{22}(OH^{-})_{2}$ and tremolite for the colourless type, while amosite is a fibrous variety of cummingtonite - grunerite ($\square(Mg^{2+},Fe^{2+})_{2}(Mg^{2+}, Fe^{2+})_{5}Si^{4+}_{8}O^{2-}_{22}(OH^{-})_{2}$) and carintnine and hornblende have been confined

to eclogite occurrences (Koritnig 1940; Binns 1967).

The derivation of a name for a mineral from its chemical analysis, usually recast as an atomic formula, involves a comparison of the unknown with compositions named according to some classification. When these named compositions represent extremes of variation in the mineral group and when any other composition can be described by a unique linear combination of positive contributions from these, the extreme compositions are referred to as end members of the group. When the number of independent chemical variables necessary to describe the chemical variation of a mineral group is small, the comparison is normally made graphically. A name is given to the unknown by noting where the analysis falls relative to named compositions. Alternatively, the unknown can be considered as a linear combination, or solid solution, of the available end member compositions. The chemical complexity of the amphiboles hinders both approaches to the naming of amphibole analyses.

Taking compositions from Deer, Howie & Zussman (1963), Perry (1967) demonstrated that it is possible to describe uniquely the chemistry of an amphibole, originally given as m oxides, in terms of a linear combination of at most m-1 amphibole compositions. However, in general, these m-1 compositions cannot be considered as end members to the amphibole group as negative contributions from one or more are required to describe the unknown. Perry (1967, 1968, 1970) has suggested that it may be possible to determine the true end members for the amphiboles but these would not obey amphibole stoichiometry. There would also be more than m+1 of these because the same cation can enter more than one structural position. As succinctness is one of the main reasons for deriving a name for a chemical analysis there seems little value in a method which requires additional variables.

Phillips & Layton (1964) and Phillips (1966) proposed an elegant chemical classification of the calciferous and alkali amphiboles. Starting from tremolite and applying six coupled ionic substitutions

(i)	$2Na = \square\ Ca$	(iv)	$Al^{vi}Al^{iv} = MgSi$
(ii)	$NaAl^{vi} = CaMg$	(v)	$CaAl^{iv} = Na\ Si$
(iii)	$\square\ Al^{vi} = NaMg$	(vi)	$NaAl^{iv} = \square\ Si$

Phillips and Layton arrived at nine extreme compositions.

(Tr)	$\square\ Ca_2\ Mg_5\ Si_8\ O_{22}\ (OH)_2$	(Pa)	$Na\ Ca_2\ Mg_4\ Al\ Si_6\ Al_2\ O_{22}\ (OH)_2$
(Ts)	$\square\ Ca_2\ Mg_3\ Al_2\ Si_6^{Al_2}O_{22}\ (OH)_2$	(Su)	$Na\ Ca\ Na\ Mg_3\ Al_2\ Si_6\ Al_2\ O_{22}\ (OH)_2$
(G)	$\square\ Na_2\ Mg_3\ Al_2\ Si_8\ O_{22}\ (OH)_2$	(Ec)	$Na\ Na_2\ Mg_4\ Al\ Si_8\ O_{22}\ (OH)_2$
(R)	$Na\ Ca\ Na\ Mg_5\ Si_8\ O_{22}\ (OH)_2$	(M)	$Na\ Na_2\ Mg_3\ Al_2\ Si_7\ AlO_{22}\ (OH)_2$
(Ed)	$Na\ Ca_2\ Mg_5\ Si_7\ AlO_{22}\ (OH)_2$		

Each of these was consistent with the generally accepted stoichiometry of the calciferous and alkali amphiboles, $0 < Na^A \leqslant 1.0$, $0 < Na^X \leqslant 2.0$, $0 \leqslant Al^{vi} \leqslant 2.0$, $0 \leqslant Al^{iv} \leqslant 2.0$.

Two of the compositions, (Su) sundiusite and (M) miyashiroite were suggested for the first time and did not correspond to known amphiboles. These names were later discredited by Fleischer (1965, 1966).

An analysis of a calciferous or alkali amphibole may be compared with the compositions if it is first converted to what Phillips and Layton termed a basic atomic formula. In its simplest form this is calculated by converting all monovalent cations in the A and X groups to equivalent Na and trivalent plus tetravalent cations in the Y group and trivalent cations in the Z group to equivalent Al. Divalent cations in the X and Y groups are returned as equivalent Ca and Mg respectively. The general form of the basic atomic formula is

$$Na^A_{0-1}\ (CaNa^X)_2\ (MgAl^Y)_5\ (SiAl^Z)_8\ O_{22}\ (OH)_2$$

and acts as a concise way of describing the overall composition of a calciferous or alkali amphibole. Phillips (1966) recognised that in any accurate analysis ($Na^{A} + Al^{Y}$) should equal ($Na^{X} + Al^{Z}$). Once any three are known the fourth is determined. Taking the three variables Na^{X}, Al^{Y}, Al^{Z} parallel to three orthogonal axes, all calciferous and alkali amphiboles lie in a defined region, termed 'amphibole compositional space' (Fig. 1.1). The nine compositions form the vertices of the space. While these vertices represent extreme amphibole and basic atomic formula compositions they are not all end members of the amphibole group since in any three dimensional representation there can be, at most, only four end members (Whittaker 1968), which will provide by a unique linear combination, the composition of any intermediate amphibole. Extreme compositions which are not true end members will be designated as 'end members'.

Phillips subdivided amphibole compositional space into nine segments (*sensu extenso* names) corresponding to the extension of the 'end members' into the space. Using such a classification an amphibole, after first recalculating to a basic atomic formula, may be described in any of three ways, (i) by its *sensu extenso* name, (ii) a combination, not unique, of the 'end members', or (iii) quoted in terms of its co-ordinates Na^{X}, Al^{Y}, Al^{Z}.

This classification is by no means the only one which has been proposed for the amphiboles, nor unfortunately is it frequently used. The subdivision of amphibole compositional space into *sensu extenso* regions has been criticised by Whittaker (1968) on the grounds that by confining the nomenclature of possible compositions to the nine 'end members' so that each *sensu extenso* region extends obliquely with reference to the co-ordinate axes, the inherent simplicity of the system has been sacrificed.

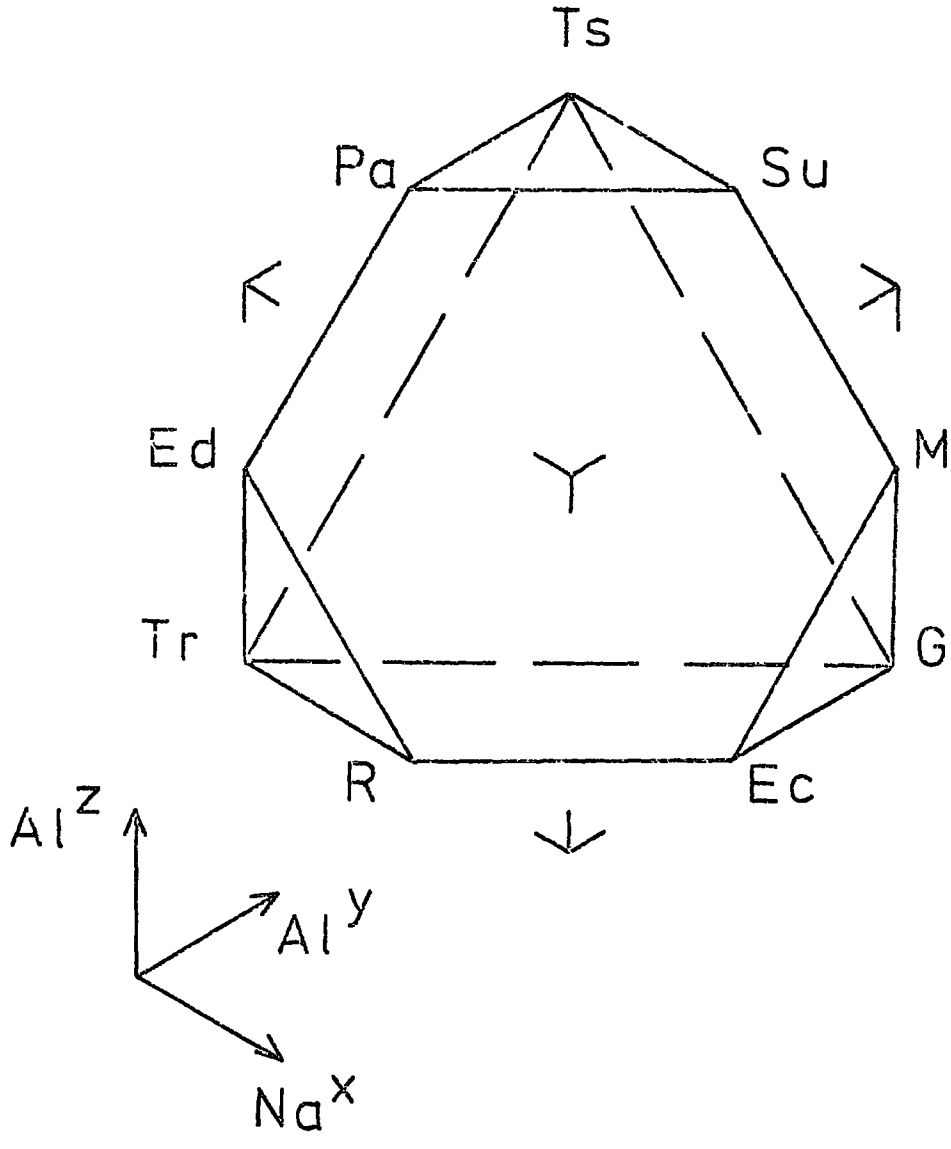


Fig 1.1. Amphibole compositional space after Phillips (1966). Abbreviations are as follows :- Tr tremolite, Ts tschermakite, G glaucophane, Ed edenite, Pa pargasite, Su sundiusite, M miyashiroite, Ec eckermannite and R richterite.

The relative merits of amphibole compositional space and topologically equivalent classifications proposed by Fabries (1966) and Whittaker (1968) will be discussed in Chapter 5. Other classifications of the calciferous (Hallimond 1943; Winchell 1945; Boyd 1959), calciferous and subcalciferous (Leake 1968) and alkali amphiboles (Miyashiro 1957) will be described relative to amphibole compositional space.

Examination of the subdivision of amphibole compositional space into sensu extenso regions, as originally suggested by Phillips (1966), revealed a number of inconsistencies. An alternative subdivision is suggested and a method whereby a calciferous or alkali amphibole may be described uniquely in terms of a linear combination of 'end members' is outlined. Using the concept of the basic atomic formula an additional three dimensional compositional space capable of showing the relationship between the calciferous, alkali and Fe/Mgln (cummingtonite-grunerite, anthophyllite, gedrite) amphiboles is described. Lastly, in Chapter 5, using a large collection of amphibole analyses, see below, the status of the discredited 'end members' miyashiroite and sundiusite and the additional 'end members' of the extended compositional space are discussed.

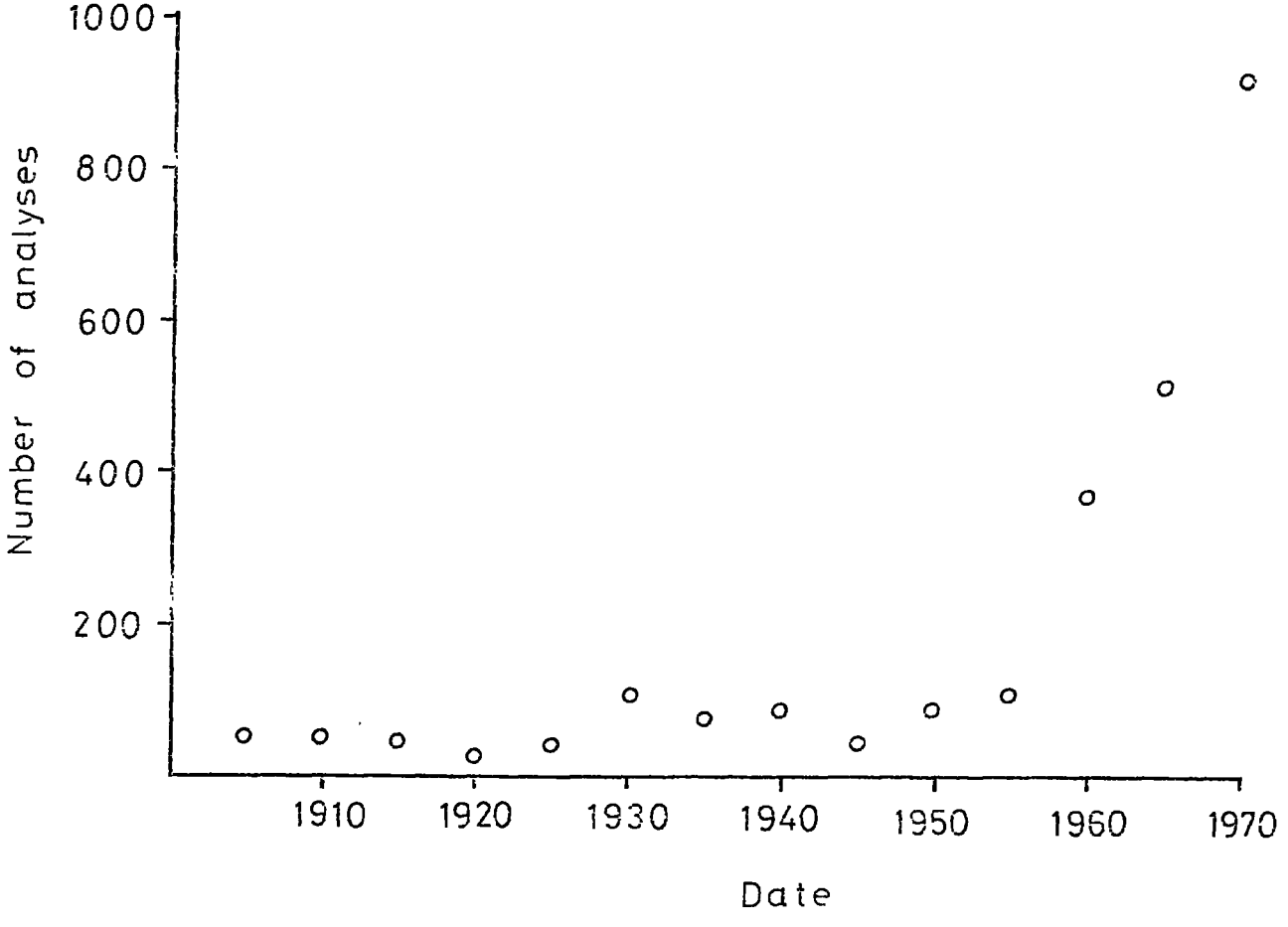
A comprehensive and representative collection of amphibole chemical analyses would be of particular value in outlining the overall chemical variation and degree of isomorphous substitution in the amphiboles as a group. Using such a collection, proposed nomenclatures and classifications of the amphiboles can be evaluated. The attention of experimental petrologists can be focused on those compositions which occur commonly in nature and on those where, possibly because of miscibility relations, amphiboles are either rare or absent. If information concerning the paragenesis of the analysed amphibole is

provided the data can be used to evaluate the significance of a newly analysed amphibole by comparing this with other similar compositions and with analyses from similar parageneses. The relationship between amphibole composition and paragenesis may also become apparent.

To these ends a number of previous workers (Eitel 1922; Kunitz 1930; Hallimond 1943; Sundius 1946; Rabbit 1948; Miyashiro 1957; Deer, Howie & Zussman 1963; Phillips & Layton 1964; Borg 1967b; Leake 1962, 1965a,b, 1968, 1971; Kostyuk & Sobolev 1969; Saxena & Ekstrom 1970; Robinson, Ross & Jaffe 1971) have accumulated analyses of amphiboles. Unfortunately, these collections were either numerically small or restricted to specific ranges of amphibole composition and as such were unrepresentative of the amphiboles as a group. In order to obtain a representative collection of amphibole analyses, data relevent to as many amphiboles as could be found in the literature were collected. It soon became apparent that the volume of data was considerable. A total of 2650 analyses were located by the middle of 1972. Like geochemical data in general (Wilkinson 1970), information concerning amphiboles is increasing at an alarming rate, see Fig. 1.2. At the same time the existence of 'type specimens' means that the total information is increasing accumulatively rather than possessing a short 'half life'. In order to cope it became obvious that a computer based data file would be required.

In Chapter 4 the merits of various data base strategies are discussed. Experience with a data base written by the author is briefly described. Thanks to the generosity of Dr M.G. Notley of the IBM United Kingdom Scientific Centre it has been possible to implement the amphibole data file under a prototype general data base strategy. The generality of this data base is demonstrated for

Fig. 1.2. Number of analyses in the amphibole data file published during successive five year intervals. The source of the data is to be found in Appendix 8.



geological data with examples taken from stratigraphy and mineralogy and in Sections 4.2 to 4.4 the implementation of the amphibole data file is described.

Atomic formulae and basic atomic formulae have been calculated for all 2650 analyses in the amphibole data file. Since this is the first time that large numbers of basic atomic formulae have been calculated, the characteristics of the charge balance achieved by natural amphiboles and various features of the method used to calculate the basic atomic formulae are discussed (Chapter 6).

Two axis plots have been used previously to illustrate the variation of either the calciferous (Hallimond 1943; Winchell 1945; Sundius 1946; Boyd 1959; Leake 1962, 1965b, 1968, 1971), alkali (Miyashiro 1957) or orthorhombic amphiboles (Rabbit 1948). In addition, Saxena & Ekstrom (1970) have used principal component analysis to investigate the substitutional replacements in the calciferous amphiboles and Robinson, Ross & Jaffe (1971) devised a method for showing how orthorhombic and calciferous amphiboles departed from the ideal 'end members' anthophyllite and tremolite respectively.

Using the three dimensional representation provided by amphibole compositional space and the additional space devised by the author, the distribution of basic atomic formulae of naturally occurring monoclinic and orthorhombic amphiboles is illustrated and described in Chapter 7. While Deer, Howie & Zussman (1963), Ernst (1968) and Whittaker (1968) have discussed the chemical variation of the amphibole group, using small numbers of analyses, it is believed that this is the first time that the major chemical variation exhibited by the amphibole group has been illustrated in a graphical

manner. From the observed distribution of basic atomic formulae the importance of proposed coupled isomorphous substitations within the amphibole structure are discussed and the possibility of a solvus or solvi within the calciferous and alkali amphiboles is investigated.

A number of workers including Hallimond (1943), Miyashiro (1957), Boyd (1959), Deer, Howie & Zussman (1963), Leake (1966, 1971), and Kostyuk & Sobolev (1969) have shown that there is a general relationship between amphibole composition and mode of occurrence. Using the basic atomic formulae and the mode of occurrence of analyses contained in the amphibole data file the nomenclature and distribution of basic atomic formulae from the major igneous and metamorphic parageneses including ultramafic - ultrabasic, basic, intermediate, acid, basic alkali, alkali igneous parageneses and eclogite, calcareous, ferruginous, serpentinite and the remaining metamorphic parageneses is described in Chapter 8. Finally, the general features of the relationships between host rock type and amphibole composition are discussed.

2. Derivation of a chemical allocation scheme for ions between groups of sites in the amphibole structure.

In order to be able to calculate an atomic formula for an amphibole from a chemical analysis it is necessary to be able to distribute the number of ions, calculated from an anion or cation base, between the crystallographic sites, or groups of sites, in the crystal structure. Phillips (1963) proposed a scheme for the allocation of ions to groups of sites in the amphibole structure. The scheme was based on crystal chemical considerations and evidence from previously determined X-ray site populations. The allocation scheme was later incorporated into an unpublished computer program entitled MINDATA3 (R. Phillips pers. comm. 1965). In MINDATA3 the numbers of ions are calculated from a chemical analysis using the anion bases of 24(O) and 23(O) and distributed between the A,X,Y,Z and hydroxyl groups (for definition of these see Chapter 1) according to the following scheme.

1) Calculate an atomic formula using anion bases of 24(O) and 23(O).

2) Allocate OH^-, F^- and Cl^- to the hydroxyl group, any excess H^+ in the analysis entering the A group. Should the sum of $OH^- + F^- + Cl^-$ be less than 2.0 the hydroxyl group is made up to 2.0 by O^{2-}, provided there is sufficient ferric iron available to balance the substitution $Fe^{2+} + OH^- = Fe^{3+} + O^{2-}$. Warnings are given if there is either insufficient ferric iron, $F^- + Cl^-$ is greater than 2.02 or $F^- + Cl^- + OH^-$ is greater than 3.03.

3) Allocate Si^{4+} to the Z group and make up to a total of 8.0 with Al^{3+}. Any remaining Al^{3+} is transferred to the Y group. Warnings are given if the total Si^{4+} exceeds 8.08 or the total $Si^{4+} + Al^{3+}$ is less than 7.95.

4) Initially allocate all Al^{VI}, Ti^{4+}, Zr^{4+}, Cr^{3+}, V^{3+}, Fe^{3+}, Li^+,

Ni^{2+}, Co^{2+}, Zn^{2+}, Mn^{2+}, Fe^{2+}, Mg^{2+} to the Y group and sum the total number of these cations. If the sum exceeds 5.05, ions are transferred to the X group in the order Mn^{2+}, Fe^{2+}, Mg^{2+}, (Mg^{2+} + Fe^{2+}), but only if the amount of/ individual cation is greater than the excess. Thus for example if the sum was 5.6 and Mn^{2+} was only 0.4, manganese would not be transferred to the X group.

5) If the sum of the Y group is less than 5.0 the possibility of vacancies associated with tetravalent or trivalent cations is considered. The substitutions Ti^{4+} + □ = $2Mg^{2+}$ and $2R^{3+}$ + □ = $3R^{2+}$ are made in the above order until the sum is raised to 5.0. If this fails to raise the Y group total to 5.0 a warning is given. In addition Li^{+} in the Y group is balanced by trivalent cations viz. $Li^{+} + Al^{3+} = 2Mg^{2+}$, $Li^{+} + Fe^{3+} = 2Mg^{2+}$.

6) If the group A is already in excess of, or equal to, 2.0 all Ca^{2+}, Ba^{2+}, Sr^{2+}, Na^{+}, K^{+}, enters the A site.

7) If the sum of the X group is less than 2.0 the group is made up to 2.0 with Ca^{2+}, Ba^{2+}, Sr^{2+}, Na^{+}, K^{+}, in that order, with any excess entering the A site.

Since the scheme was derived in 1963 the number of published site populations of amphiboles has increased greatly due to the advent of infrared and Mössbauer spectroscopy. In addition amphiboles with appreciable amounts of cations not included in Phillips' scheme, for example, cobalt in Na - Co amphibole (Gier, Cox & Young 1964), lead and beryllium in joesmithite (Moore 1969), have been described. It therefore seemed appropriate to re-examine the allocation scheme employed in MINLATT3 and to extend and amend this in the light of recent information/ site populations. The reader unfamiliar with the techniques of X-ray diffraction, infrared and Mössbauer spectroscopy for determining cation distributions is referred to Appendix 2.

In order to check the allocation scheme employed in MINDATA3 the group populations of cations, calculated from chemical analyses alone, were compared with published experimentally determined cation distributions for the same specimens. The comparison was made between groups of sites, for all the published experimentally determined cation distributions (complete or partial) the author was aware of, provided a chemical analysis was also available for the investigated material. Where the experimentally determined cation distribution was given for cations between individual sites, group populations were derived by summing the content of individual cations in the sites comprising a group to facilitate direct comparison with calculated group populations of MINDATA3. Appendix 3 lists the source and experimentally determined cation distributions of the specimens used plus the cation group populations calculated for the same specimens from their analyses using MINDATA3 and the amended allocation scheme incorporated in MINDATA5 (see below). Since this was written a number of additional site populations have come to the author's attention but are not included in Appendix 3. These include Litvin, Yegoreva & Repikin (1971), Kitamura & Morimoto (1972). Litvin, Yegoreva & Kuts (1972), Kamineni (1973), Litvin Michnik & Ostapenko (1973), Mixitina, Petkevich & Sverdlova (1973), Sueno, Cameron, Papike & Prewitt (1973), Finger & Ohashi (1974) and Seifert & Virgo (1974).

While it is difficult to interpret the results of such an approach since there may be errors in the original analysis, the allocation scheme and the published site populations (Appendix 2), it become apparent that the calculated and experimentally determined populations at group level differed in a systematic manner, Section 2.1. Using the observed site populations an amended allocation scheme was derived in Section 2.2 and extended to include additional

cations by crystal chemical considerations, Section 2.3. This allocation scheme was incorporated into a computer program entitled MINDaTa5, Section 2.4, the results of which (see Appendix 3) were compared with known site populations, Section 2.5.

2.1. Evaluation of MINDaT13.

Four measures were employed to express the similarity between the experimentally determined and calculated group populations. Firstly a simple measure of the difference between the experimentally determined and calculated value of each cation in a group of sites.

(1) ---- $$Sa = I^{i}_{calc.} - I^{i}_{ex.det.}$$

where

$I^{i}_{calc.}$ = calculated value for cation I, in group i.

$I^{i}_{ex.det.}$ = experimentally determined value for cation I in group i.

Sa should approach zero as the similarity between the experimentally determined and calculated values increases.

To measure the similarity between the calculated and experimentally determined values for all the cations in an analysis measure Sb was employed.

(2) ---- $$Sb = \frac{\sum_{1-M}^{I} \sum_{1-N^{I}}^{i} \left| I^{i}_{calc.} - I^{i}_{ex.det.} \right|}{\sum_{1-M}^{I} N^{I}}$$

where

$I^{i}_{calc.}$, $I^{i}_{ex.det.}$ are as (1)

M = total number of cations for which a comparison is being made,

N^I = total number of groups in which cation I is found.

Measure Sb may be considered the mean absolute difference between the calculated and experimentally determined populations for all the cations over all groups for one specimen. Sb can only take positive values. For a good agreement between experimentally determined and calculated values Sb approaches zero.

Both Sa and Sb are dependent on the amount of cation present in a group and as such are dependent on the recalculation base used. They are affected if a different recalculation base has been used in calculating the number of cations in I^i_{calc} from that used for $I^i_{ex.det.}$. As a partial solution to this complication two additional measures Sc and Sd were defined.

After normalising for the site multiplicity of the groups, the ratio of a cation in one group compared with the total of the same cation in all groups yields a ratio indicating the ordering of the cation.

$$(3) \text{ ----} \quad R_{Ii} = \frac{I^i/m^i}{\sum_{1-N^I}^{i} I^i/m^i}$$

Where

I^i = value for cation I in group i.

m^i = site multiplicity of group i.

N^I = the number of groups cation I is found in.

The ratio equals 1.0 if I is ordered into one group, 0.0 if absent from a group and 0.5 if randomly ordered between two groups. For comparative purposes measure Sc may be defined.

(4) ---- $Sc = R_{Ii}^{calc.} - R_{Ii}^{ex.det.}$

where

$R_{Ii}^{calc.}$ and $R_{Ii}^{ex.det.}$

are the ordering factors for cation I in group i derived from the calculated and experimentally determined cation distributions.

Values close to zero indicate a close comparison between the experimentally determined and calculated distribution of a cation.

lastly measure Sd was defined.

(5) ---- $$Sd = \frac{\sum_{1-M}^{I} \sum_{1-N^I}^{i} \left| R_{Ii}^{calc.} - R_{Ii}^{ex.det.} \right|}{\sum_{1-M}^{I} N^I}$$

where

$R_{Ii}^{calc.}$, $R_{Ii}^{ex.det.}$ are as (4),

M, N^I are as (2).

Sd is the mean absolute difference between the calculated and experimentally determined ordering factors for all the cations over all the groups for one specimen. It bears the same relation to Sc as measure Sb does to Sa. The measure can only take positive values.

Using MINDATA3 group populations were calculated for each of the analyses included in Appendix 3. In every case a recalculation base of 23(O) was used. For those analyses with either H_2O+, F or Cl determined group populations were also calculated to 24(O). The resultant group populations are listed in Appendix 3. Using these calculated values and the experimentally determined cation distributions values for the four measures were derived.

In order to illustrate the extent of the agreement between the calculated and experimentally determined group populations a number of statistics and diagrams were used.

The statistics,

n, the number of values,

$\bar{x}$, the arithmetic mean,

σ, the standard deviation,

$|\bar{x}|$, the mean deviation from zero,

of measures Sa and Sc for each cation in each group are given in Tables 2.1 and 2.2. The mean deviation from zero was introduced because an arithmetic mean near zero does not necessarily imply that values for Sa and Sc are small since equal numbers of large positive and negative deviations could also yield an arithmetic mean near zero. Histograms of measures Sb and Sd are given in Figs. 2.1 and 2.2. Values for Be^{2+} in Z, Pb^{2+}, Ca^{2+} in A (joesmithite), Co^{2+} in X,Y (Na - Co amphibole) and Li^{+} in A (protoamphibole) which were outside the scope of MINDAT.3 have been omitted.

The histograms demonstrate that for the majority of compositions included in appendix 3 the differences between the experimentally determined and calculated group populations were small. However, a number of analyses have values for Sb or Sd in excess of 0.5. With regard to measure Sb this represents an average discrepancy of 0.5 for each cation in each group. For measure Sd, a value in excess of 0.5 indicates a considerable discrepancy in the ratio of cations between groups. These analyses include anthophyllite, (2,3), holmquistite, (6), cummingtonite - grunerite, (9, 27, 38, 42) and two tremolites (45,53), (see Appendix 3 for further details). An examination of these analyses suggested that the discrepancy could be attributed to errors in the sequence in which cations normally present in the Y group enter the X group (M4 sites) when the sum of

Table 2.1. Statistics of measure Sa calculated using MINDATA3.

cation	group	24(O) $\bar{x}$	24(O) σ	24(O) $\lvert\bar{x}\rvert$	24(O) n	23(O) $\bar{x}$	23(O) σ	23(O) $\lvert\bar{x}\rvert$	23(O) n
Si^{4+}	Z	0.0744	0.231	0.132	9	0.018	0.263	0.150	9
Al^{iv}	Z	-0.007	0.067	0.058	7	0.061	0.086	0.070	7
Ti^{4+}	Y	0.036	0.073	0.044	7	0.028	0.071	0.037	7
Al^{vi}	Y	-0.024	0.075	0.054	13	-0.083	0.105	0.085	13
Fe^{3+}	Y	0.018	0.115	0.081	22	0.023	0.115	0.082	22
Fe^{2+}	Y	-0.057	0.371	0.227	46	-0.055	0.331	0.201	76
Mn^{2+}	Y	-0.140	-	0.140	1	-0.200	-	0.200	1
Mg^{2+}	Y	-0.192	0.564	0.311	26	-0.143	0.426	0.256	27
Fe^{2+}	X	0.020	0.408	0.262	24	-0.010	0.359	0.225	48
Mn^{2+}	X	-0.196	0.403	0.268	5	-0.198	0.406	0.270	5
Mg^{2+}	X	0.264	0.585	0.450	14	0.202	0.564	0.429	15
Li^{+}	X	-1.150	0.650	1.150	2	-1.150	0.650	1.150	2
Ca^{2+}	X	-0.023	0.106	0.051	18	-0.024	0.108	0.049	18
Na^{+}	X	0.013	0.233	0.136	15	0.027	0.210	0.104	15
K^{+}	X	-0.020	-	0.020	1	-0.020	-	0.020	1
Na^{+}	A	-0.030	0.119	0.103	6	-0.058	0.168	0.121	6
K^{+}	A	0.000	0.014	0.010	4	0.010	0.035	0.025	4

Table 2.2. Statistics of measure Sc calculated using MINDATA3.

Cation	Group	24(O) $\bar{x}$	24(O) σ	24(O) $\lvert\bar{x}\rvert$	24(O) n	23(O) $\bar{x}$	23(O) σ	23(O) $\lvert\bar{x}\rvert$	23(O) n
Si^{4+}	Z	0.00	0.00	0.00	8	0.00	0.00	0.00	8
Al^{iv}	Z	-0.006	0.118	0.072	11	0.069	0.086	0.078	11
Ti^{4+}	Y	0.011	0.028	0.011	7	0.011	0.028	0.011	7
Al^{vi}	Y	-0.068	0.279	0.131	14	-0.129	0.253	0.136	14
Fe^{3+}	Y	0.00	0.00	0.00	21	0.00	0.00	0.00	21
Fe^{2+}	Y	-0.078	0.319	0.184	47	-0.065	0.267	0.142	75
Mn^{2+}	Y	-0.040	-	0.040	1	-0.050	-	0.050	1
Mg^{2+}	Y	-0.039	0.168	0.109	25	-0.003	0.157	0.093	26
Fe^{2+}	X	-0.064	0.320	0.209	18	-0.046	0.202	0.100	39
Mn^{2+}	X	-0.525	0.479	0.545	4	-0.560	0.456	0.585	4
Mg^{2+}	X	0.055	0.227	0.191	13	0.025	0.212	0.172	14
Li^{+}	X	-0.895	0.105	0.895	2	-0.895	0.105	0.895	2
Ca^{2+}	X	-0.081	0.231	0.080	18	-0.014	0.055	0.014	18
Na^{+}	X	-0.204	0.415	0.268	15	-0.104	0.246	0.136	15
K^{+}	X	0.0	-	0.0	1	0.0	-	0.0	1
Na^{+}	A	-0.073	0.091	0.083	6	-0.075	0.101	0.078	6
K^{+}	A	0.00	0.00	0.00	4	-0.040	0.069	0.040	4

Fig. 2.1. Histograms of the measure Sb.

(a) Calculated values taken from MINDATA3, recalculation base 24(O), 53 analyses. Protoamphibole (7), Na - Co amphibole (68) and joesmithite (69), see Appendix 3, have been excluded as these analyses lay outside the original scope of MINDATA3.

(b) Calculated values taken from MINDATA5, recalculation base 24(O), 56 analyses.

(c) Calculated values taken from MINDATA3, recalculation base 23(O), 83 analyses. Values for analyses (7, 68, 69, Appendix 3) have been excluded, see (a).

(d) Calculated values taken from MINDATA5, recalculation base 23(O), 86 analyses.

The hatched column represents the number of analyses with values of Sb in excess of 0.5.

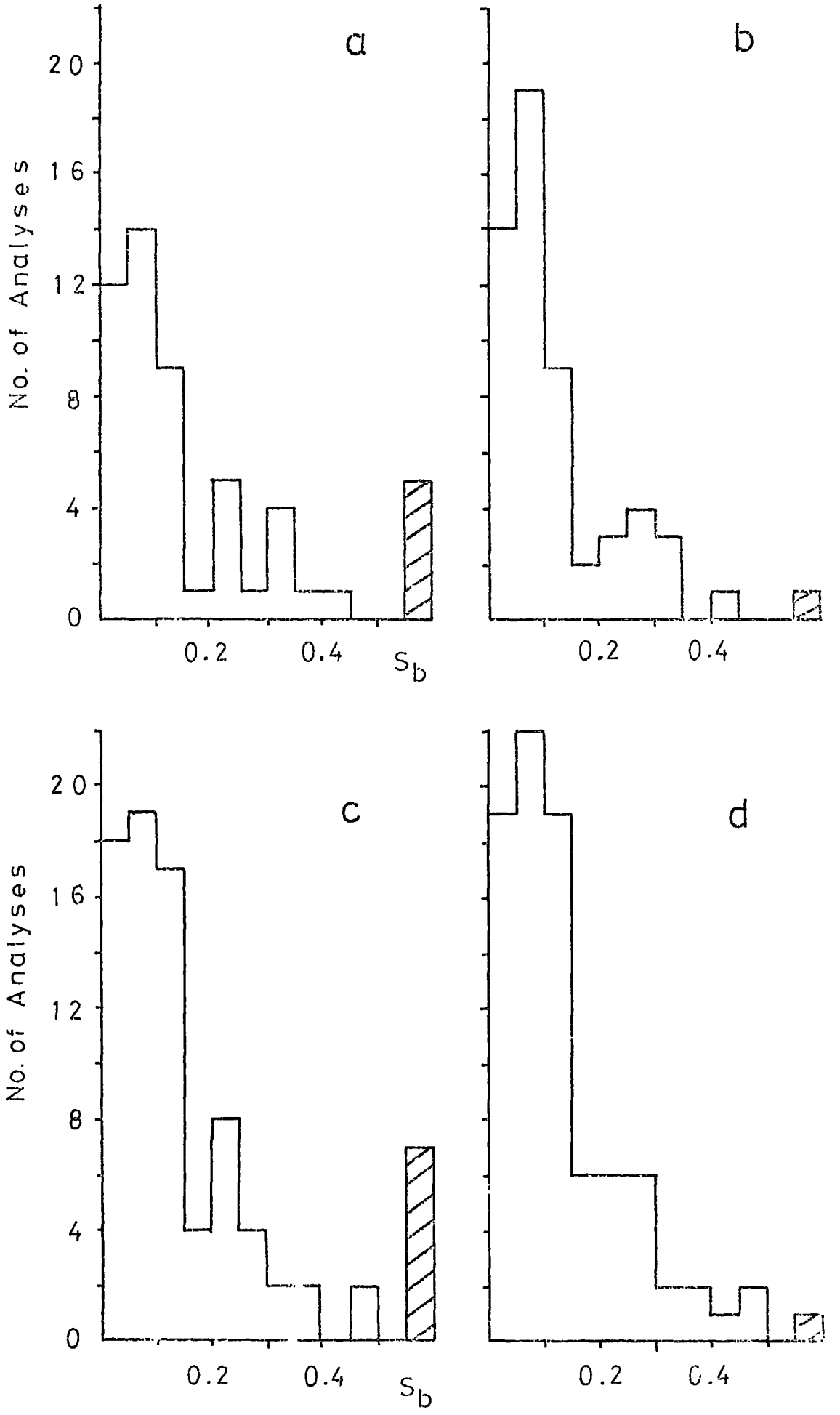

a
b
c
d
No. of Analyses
20
16
12
8
4
0
0.2
0.4
s_b

Fig. 2.2. Histograms of the measure Sd.

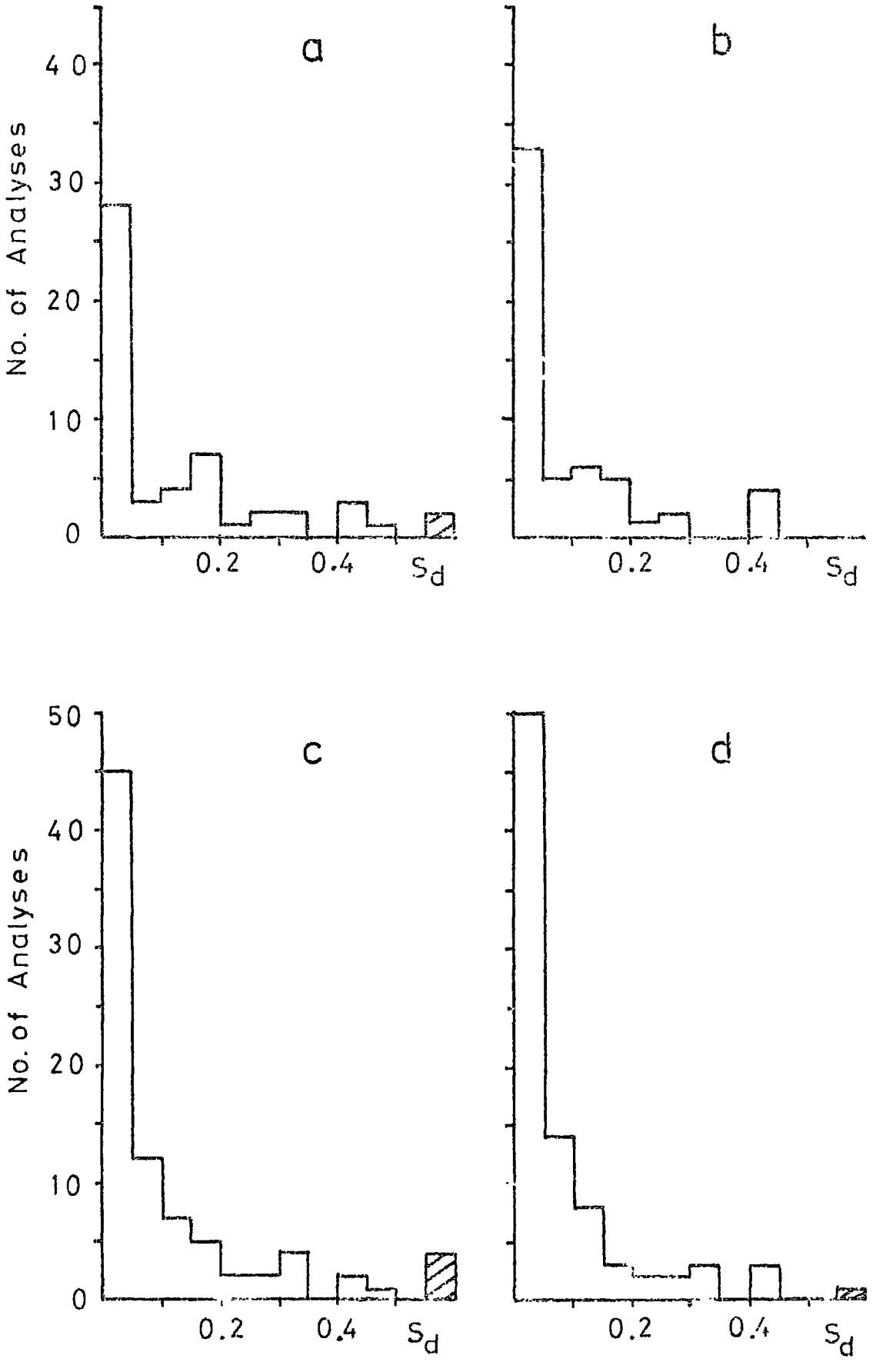
(a) Calculated ratios taken from MINDATA3, recalculation base 24(0), 53 analyses. Protoamphibole (7), Na - Co amphibole (68) and joesmithite (69), see Appendix 3, have been excluded as these analyses lie outside the original scope of MINDATA3.

(b) Calculated ratios taken from MINDATA5, recalculation base 24(0), 56 analyses.

(c) Calculated ratios taken from MINDATA3, recalculation base 23(0), 83 analyses. Values for analyses (7, 68, 69 Appendix 3) have been excluded, see (a).

(d) Calculated ratios taken from MINDATA5, recalculation base 23(0) 86 analyses.

The hatched column represents the number of analyses with values for Sd in excess of 0.5.


a
b
c
d
No. of Analyses
40
30
20
10
0
50
0.2
0.4
S_d

Si^{4+}, Al^{3+} Fe^{3+} Ti^{4+}, Fe^{2+}, Mg^{2+}, Mn^{2+}, Li^{+} excedes 13.0.

Similarily an inspection of the statistics for measure Su and Sc, (Tables 2.1, 2.2), reveals numerically small values for $\bar{x}$, σ and $|\bar{x}|$ for nearly all the cations. (Identical experimentally determined and calculated group populations will yield values of zero for all three statistics.) In detail the statistics for certain of the cations deviate considerably from zero. This applies in particular to Fe^{2+}, Mg^{2+}, Mn^{2+}, in both the Y and X groups, and Li^{+} in the X group which again suggests that the main difference between the experimentally determined and calculated group populations involves those cations which can occupy sites in both the Y and X groups.

Using the experimentally determined cation distributions it has proved possible to amend and extend the allocation scheme of MINDAT3.

2.2. Derivation of a generalised allocation scheme at group level from experimentally determined site populations.

An allocation scheme has been constructed from experimentally determined cation distributions, by assuming that the ordering factor (R_{I}^{cy}.det.) of a cation in a group reflects the preference of the cation for the group. Natural and synthetic amphiboles belonging to the space groups C2/m, $P2_1/m$, P2/a, Pnma, and Pnmn have been included in the construction of the scheme. The situation is complicated by variation of ordering factors with bulk chemistry and possibly the temperature of crystallisation.

In deriving the allocation scheme the distribution of cations between sites within individual groups, for example between the M1, M2 and M3 sites of the Y group, was not taken into account. For most purposes an atomic formula at group level is satisfactory.

At the same time this greatly simplifies the calculation of the atomic formula since there is increasing evidence (Prentice 1967; Burns & Prentice 1968; Bancroft & Burns 1969; Ernst & Wai 1970; Burns & Greaves 1971; Litvin et al. 1972) that ordering within the Y group may be related to the physical conditions of formation as well as the chemistry of the mineral.

To enable a group population to be calculated from a chemical analysis alone, possible variation in ordering as a function of temperature of crystallisation has to be neglected. A consideration of variation of order - disorder at group level as a result of this factor will be deferred until Section 2.5.

In Table 2.3 the ranges of the ordering factors $R_{I}^{ex.det.}_{i}$ for the major cations between groups of sites are tabulated. Inspection reveals that only Si^{4+}, Be^{2+} and Pb^{2+} are consistently ordered into a single group. Data for Be^{2+} and Pb^{2+} are taken from a single X-ray population for the unique amphibole, joesmithite (Moore 1969). The remaining cations are either not fully ordered into one group, or alternatively, show a range of ordering with bulk chemistry. The single values for Al^{3+}, Ti^{4+} and Fe^{3+} in the X group are all taken from the same X-ray refinement of a kaersutite by Kitamura & Tokonami (197 in which Fe^{2+}, Fe^{3+}, Al^{3+}, Mg^{2+} and Ti^{4+} in the X group were not distinguished. Because of this it is tentatively suggested that none of these three occupy a site in the X group.

2.2.1. Z group.

Taking the Z group first. All Si^{4+} may be allocated to the group. Any Be^{2+} is tentatively assigned to the group also. The only remaining cation reported from the group in the site populations in Appendix 3 is aluminium. It is common practice (Leake 1968) to

Table 2.3. Range of ordering factors (ex.det) for cations between groups of sites. The source of data is taken from published experimentally determined cation distributions in Appendix 3. The number of cation distributions on which each range is based is shown in parenthesis.

on	Amphibole type*	Group A	Group X	Group Y	Group Z
Si^{4+}	O,C. M	-	-	-	1.00(8)
Be^{2+}	M	-	-	-	1.00(1)
Al^{3+}	O	-	-	0.52-0.97(3)	0.03-0.48(3)
	C	-	-	0.23(1)	0.77(1)
	M	-	0.01(1)	0.15-1.0(10)	0.50-1.00(7)
Ti^{4+}	M	-	0.08(1)	0.92-1.00(7)	-
Fe^{3+}	C	-	-	1.00(1)	-
	M	-	0.11(1)	0.89-1.00(20)	-
Fe^{2+}	O	-	0.59-0.84(4)	0.16-1.00(4)	-
	C		0.45-1.00(35)	0.00-0.55(35)	-
	M	-	0.0 -0.11(36)	0.89-1.00(36)	-
Mn^{2+}	C	-	0.88-1.00(3)	0.00-0.12(3)	-
	M	-	0.00-1.00(4)	0.00-1.00(4)	-
Mg^{2+}	O	-	0.13-0.45(5)	0.55-0.87(5)	-
	C	-	0.03-0.22(5)	0.78-0.97(5)	-
	M	-	0.00-0.17(4)	0.83-1.00(16)	-
Co^{2+}	M	-	0.28(1)	0.72(1)	-
Li^{+}	O	0.79(1)	0.21-1.00(2)	-	-
	M	-	-	1.00 +	-
Ca^{2+}	O	-	1.00(2)	-	-
	C	-	1.00(3)	-	-
	M	0.38(1)	0.62-1.00(13)	-	-
Na^{+}	O	0.0-0.98	0.02-1.00(3)	-	-
	C	..	1.00(2)	-	-

	M	0.00-1.00(3)	0.00-1.00(10)	-	-
+	M	0.0-1.00(5)	1.00(1)	-	-
b^{2+}	M	1.00(1)	-	-	-

* Amphibole types are abbreviated as follows; O = orthorhombic, C = monoclinic, Fe^{2+}Mg, Mn rich amphiboles eg cummingtonite - grunerite and, M = monoclinic calcium and sodium rich amphiboles.

+ Data not included in Appendix 3, see text.

complete the Z group to 8.0 atoms with aluminium and this has been followed in the present work.

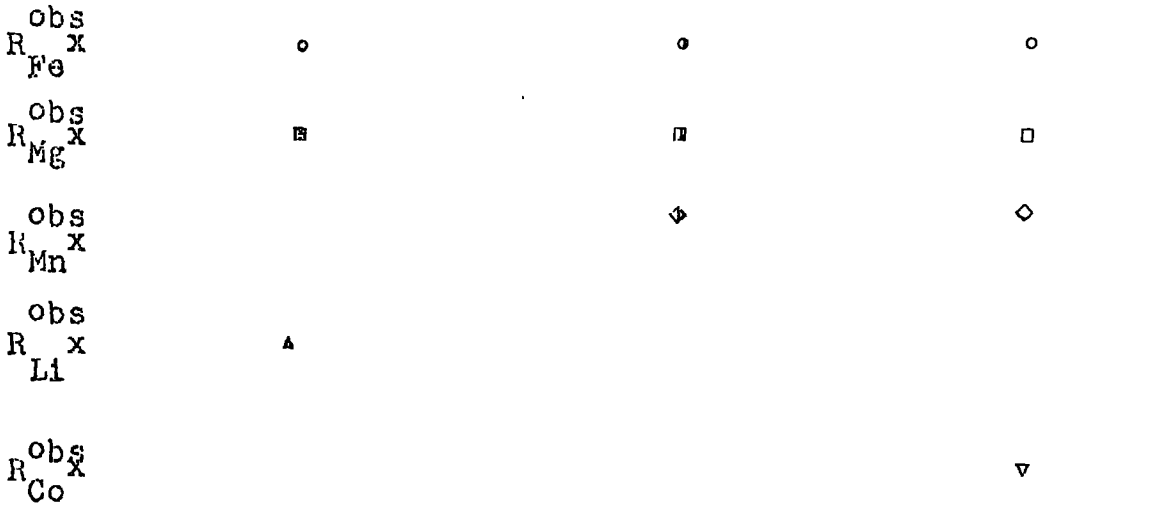
2.2.2. Y group.

From Table 2.3 it can be seen that Al^{3+}, Fe^{3+}, Ti^{4+}, Fe^{2+}, Mn^{2+}, Mg^{2+}, Co^{2+}, and Li^{+} have been reported from the Y group. With the exception of Fe^{3+}, Ti^{4+} and the remaining aluminium (Al^{vi}), the same cations have also been reported from the X group (M4 sites) for those compositions in which the sum Al^{vi}, Fe^{3+}, Ti^{4+}, Fe^{2+}, Mn^{2+}, Mg^{2+}, Co^{2+}, Li^{+} exceeds 5.0, (i.e. $\sum Y > 5.0$), see Fig 2.3. Only ferric iron, titanium and the remaining aluminium may be allocated to the Y group directly.

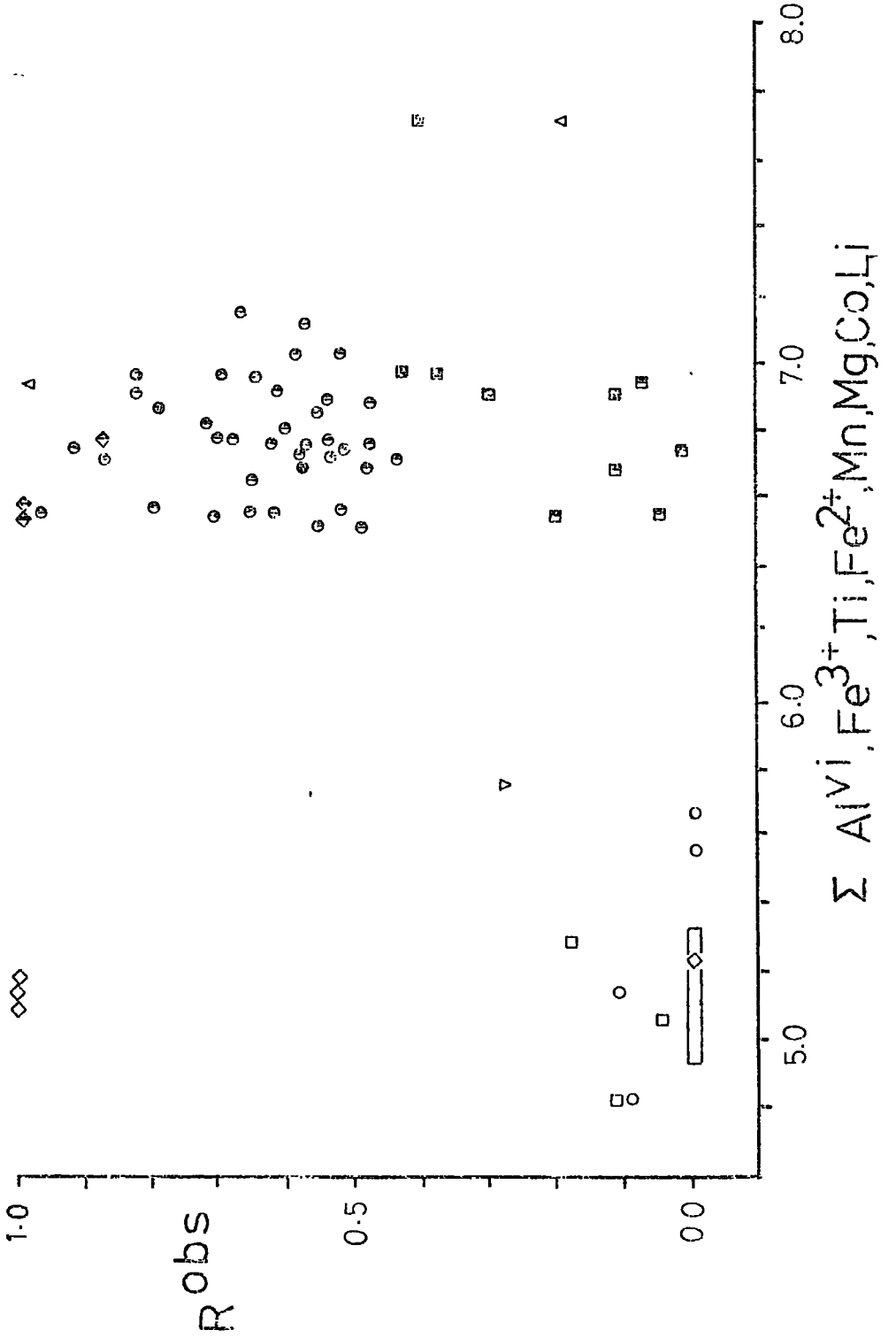
Reference to Table 2.3 shows that for the monoclinic amphiboles, other than cummingtonite - grunerite, the ordering factors for Fe^{2+}, Mg^{2+}, Co^{2+} and Li^{+} in the X group are either small or zero. This may be interpreted as a preference of the above cations for the Y group for those bulk chemistries in which the sum Al^{vi}, Fe^{3+} Ti^{4+}, Fe^{2+}, Mn^{2+}, Mg^{2+}, Co^{2+}, Li^{+} is less than or equal to 5.0 atoms, ($\sum Y \leqslant 5.0$).

Magnesium and ferrous iron are normally accepted as occupants of the Y group as is cobalt in Na - Co amphibole (Gibbs 1966). As far as the author is aware the distribution of Li^{+} has been reported for only two clinoamphiboles, both riebeckites (Colville & Gibbs 1964; data taken from Gibbs 1966; Addison & White 1968). In both these analyses Li^{+} was found in the Y group confirming the prediction of Phillips (1963). However, Whittaker (1971) has suggested from a consideration of Madelung energies, that any Li^{+} ion should show a preference for the M4 site in hydroxy and oxy clinoamphiboles. Presumably this preference refers to the larger and quantitavly more important Na^{+} ion. Here

Fig. 2.3. Variation of the ordering factors, R_{Fe}^{x}, R_{Mg}^{x}, R_{Mn}^{x}, R_{Li}^{x}, and R_{Co}^{x} with the sum of the cations normally present in the Y group (Al^{iv}, Fe^{3+}, Ti^{4+}, Mn^{2+}, Mg^{2+}, Co^{2+}, Li^{+}).



The low value for $R_{Li}^{ex\text{-}det\ x}$ at $\sum Y = 7.7$ refers to proto-amphibole in which Li^{+} has been reported from the A group in addition to the X group. The ═══ at R = 0.0 represents overlapping $R_{Fe}^{ex\text{-}det\ x}$, $R_{Mg}^{ex\text{-}det\ x}$ = 0.0 for large numbers of monoclinic Ca, Na amphiboles which could not be shown individually on the figure.


1·0
0·5
0·0
R obs
5.0
6.0
7.0
8.0
Σ AlVi, Fe3+, Ti, Fe2+, Mn, Mg, Co, Li

Li^+ has been taken as an occupant of the Y group for those compositions in which $\sum Y \leqslant 5.0$ atoms. (See also Robinson, Ross & Jaffe 1971).

Manganese has been reported to be ordered completely into the Y group of a riebeckite (Papike, Ross & Clark 1969), but in three other clinoamphiboles (Mitchell et al. 1971; Hawthorne & Grundy 1973a,b) Mn^{2+} is reported from the X group. In these three compositions $\sum Y$ exceeds 5.0 atoms and the total number of Mn^{2+} ions is small. It has been assumed that Mn enters the Y group for those compositions in which $\sum Y \leqslant 5.0$ atoms.

Based on the above considerations an allocation scheme for the Y group applicable to those compositions in which $\sum Y \leqslant 5.0$, may be inferred as :-

$$Al^{VI} = Fe^{3+} = Ti^{4+} \geqslant Mg^{2+} \geqslant Fe^{2+} \geqslant Co^{2+} \geqslant Mn^{2+} \geqslant Li^{+}$$

2.2.3. A and X groups.

Calcium is restricted to the X group for a wide range of compositions. This is in accordance with theoretical considerations of Whittaker (1971). The only exception is joesmithite in which the Ca^{2+} content exceeds the total for the X group and the excess enters the A group. Both Na^+ and K^+ have been recorded in the X group. It is generally accepted that the smaller Na^+ shows a preference for the smaller M4 co-ordination polyhedra (see Section 2.3), only entering the A group when the X group becomes full. The allocation scheme for the X group may be inferred as $Ca^{2+} > Na^+ > K^+$. In addition, Pb^{2+} has been recorded from the A site of joesmithite.

Considering the cummingtonite - grunerites, Na - Ca amphibole and the orthorhombic amphiboles gedrite, holmquistite, anthophyllite and protoamphibole in which the sum of the cations normally present in the X group exceeds 5.0, approaching 6.0 in the protoamphibole,

the excess of cations normally present in the Y group are found to enter the X group (M4 sites) in a fairly well defined sequence. X-ray and Mössbauer evidence (1) indicate that the ordering of Fe^{2+} into the X group is greater than random (Fig 2.3), while Mn^{2+} in manganese rich cummingtonites (Bancroft, Burns & Maddock 1967a; Papike, Ross & Clark 1969) is even more highly ordered into the X group than Fe^{2+}, (Fig. 2.3). On the other hand Mg^{2+} and Co^{2+} are ordered into the Y group. While, with the exception of Mn^{2+}, it is exceptional for these cations to be ordered completely into the X group and therefore absent from the Y group (Fig 2.3) an order of preference for the X group has been inferred from the observed ordering factors as $Mn^{2+} \gg Fe^{2+} > Co^{2+} \geqslant Mg^{2+}$.

In holmquistite (Whittaker 1969; Wilkins, Davidson & Ross 1970; Law 1973) Li^{+} is found exclusively in the X group (M4 sites). Wilkins et al. report Mn^{2+} present in the Y group of the holmquistite they investigated suggesting a preference for the X group (M4 sites) of $Li^{+} > Mn^{2+} \gg Fe^{2+} > Co^{2+} \geqslant Mg^{2+}$. However in the holmquistite investigated by Whittaker (1969) and Law (1973) magnesium and not iron was found with lithium in the X group. Despite this discrepancy the above scheme whereby cations are transferred from the Y to the X group has been employed.

In accordance with Phillips (1963) an error of up to 1 per cent in the Y group total is allowed. For analyses in which the

---

1). Ghose & Hellner (1959), Ghose (1961), Bancroft, Burns, Maddock & Strens (1966), Fischer (1966), Bancroft, Burns & Maddock (1967a), Finger & Zoltai (1967), Whitfield & Freeman (1967), Finger (1969), Papike, Ross & Clark (1969), Papike & Ross (1970), Buckley & Wilkins (1971), Hafner & Ghose (1971), Seifert & Virgo (1974).

sum of the Y group exceeds 5.05 atoms, cations should be transferred to the X group in the order outlined above until the sum is reduced to 5.0 atoms.

Lastly, for protoamphibole in which the sum of the cations normally present in the Y group exceeds 7.0 ($\sum Y > 7.0$) both the Y and X groups are fully occupied. In accordance with Gibbs (1966) excess Li^{+} is transferred to the A group.

2.3. Extension of the allocation scheme to include cations and bulk compositions for which no relevant experimentally determined site population data are available.

In the previous section an allocation scheme was outlined which complied with observed distributions of M4 cations. While these may be termed major cations in amphibole chemistry (Pb^{2+}, Be^{2+}, Co^{2+} excluded) they are by no means exhaustive. An examination of the analyses included in the amphibole data file (see Chapter 4), revealed that 49 cations had been recorded. Most of these only occur in trace amounts (As^{5+}, Bi^{3+}, Ce^{3+}, Dy^{3+}, Er^{3+}, Eu^{3+}, Fr, Ga^{3+}, Gd^{3+}, Ho^{3+}, La^{3+}, Lu^{3+}, Nb^{3+}, Nd^{3+}, Mo^{3+}, Pr^{3+}, Rb^{+}, Sb^{5+}, Sc^{3+}, Sm^{3+}, Sn^{4+}, Tb^{3+}, Y^{3+}, Yb^{3+}), but a number must be considered as potential components of the amphibole structure. These include B^{3+}, Ba^{2+}, Cd^{2+}, Cr^{3+}, Cu^{2+}, Ni^{2+}, P^{5+}, Sr^{2+}, V^{3+}, Zn^{2+}, Zr^{4+}. In the present work the allocation scheme was extended to include these latter cations.

Starting from the experimentally determined cation distributions it has been assumed that cations of similar size and charge would, if present, occupy similar co-ordination polyhedra and hence groups in the amphibole structure. The ionic radii of Whittaker & Muntius (1970) have been used.

The sites of the T group are at the centres of slightly distorted oxygen tetrahedra (Appendix 1). Only Si^{4+}, Al^{3+} and

Be^{2+} have been recorded from the Z group, Table 2.3, Appendix 3 . Boron, phosphorus and ferric iron may be considered as possible occupants of the group.

Ionic Radii (Å) in 4 fold co-ordination.

observed cations		possible additional cations	
Al^{3+}	0.47	Fe^{3+}	0.57
Be^{2+}	0.35		
Si^{4+}	0.34		
		P^{5+}	0.25
		B^{3+}	0.20

Synthetic boron amphiboles (Kohn & Comeforro 1955; Saito 1963) probably contain B^{3+} in the Z group. Phosphorus normally only occurs in trace amounts, but reports of larger values may often be attributed to impurities (Koritnig 1965). For the present purposes P^{5+} has been included as a possible occupant of the Z group but its presence should, it is suggested, be carefully checked. X-ray evidence for Fe^{3+} in the Z group has been proposed by Colville & Gibbs (1964). In addition, Ernst & Wai (1970) interpreted an extra doublet in the Mössbauer spectrum of a natural magnesioriebeckite as evidence of Fe^{3+} in the Z group. Ferric iron does not gain a net crystal field stabilisation energy (C.F.S.E.) in either octahedral or tetrahedral configuration (Burns 1970). It is suggested that evidence for Fe^{3+} in the Z group remains inconclusive. Until further data are forthcoming ferric iron has not been included in the Z group.

Titanium, has on occasion been included in the Z group. However, Hartman (1969) has pointed out that Ti^{4+} has only been found in a single compound, Ba_2TiO_4. C.F.S.E. is higher for Ti^{4+} in an octahedral rather than tetrahedral configuration (Dunitz & Orgel 1957).

The cation is a more appropriate occupant of the Y group.

The Y group cations are approximately central in slightly distorted octahedral co-ordination polyhedra (Appendix 1). Zn^{2+}, Cu^{2+}, V^{3+}, Cr^{3+} Ni^{3+}, Zr^{4+} have appropriate ionic radii and charges. Cu^{2+}, Cr^{3+}, V^{3+}, Ni^{2+} and Zr^{4+} have been detected frequently but in only small concentrations (for example, Dodge & Ross 1971; Roonwall 1972). Zinc, has been reported as a major component in somewhat unusual amphiboles (Bauer & Berman 1930; Fosberg 1936; Hawthorne & Grundy 1973c). Phillips (1963) suggested Y group vacancies may occur associated with charge balancing substitutions such as :-

$$Ti^{4+} + \square = 2Mg^{2+}, \quad 2R^{3+} + \square = 3R^{2+}.$$

where appropriate such substitutions may also be included.

The co-ordination polyhedra around the M4 sites forming the X group vary with bulk chemistry of the amphibole. In the calciferous and alkali amphiboles and joesmithite they are 8 fold co-ordinated while 6 fold co-ordination is found in the C2/m, P21/a cummingtonites, protoamphibole, gedrite and holmquistite. Finger (1970a,b) reported 7 fold co-ordination around the M4 sites in anthophyllite.

Considering the 8 fold co-ordinated group first, the following additional cations appear appropriate.

Ionic radii (Å) in 8 fold co-ordination.

observed cations		possible additional cations	
?K^{+}	1.59		
		?Ba^{2+}	1.50
		Pb^{2+}	1.37
		$Sr2^{+}$	1.33

Na^{+}	1.24
Co^{2+}	1.20
Cd^{2+}	1.15
Ca^{2+}	1.08
Mn^{2+}	1.01

Barium and strontium are occasionally detected in small concentrations and may be considered collectively with calcium for most purposes. Amphiboles have been synthesised with Cd^{2+} probably in the X group (Saito 1963; Fedoseev et al. 1970). Lead is also included as a possible cation in the X group.

In the 6 fold co-ordinated M4 site the occupants closely resemble those of the Y group (Na^{+}, Ca^{2+} excluded). In a sense the M4 sites (X group) may be considered as an extended Y group (Phillips 1963).

Ionic radii (Å) in 6 fold co-ordination.

observed cations		possible additional cations	
Na^{+}	1.10		
Ca^{2+}	1.08		
		Cd^{2+}	1.03
Mn^{2+}	0.91		
Fe^{2+}	0.86		
Co^{2+}	0.83		
		Zn^{2+}	0.83
Li^{+}	0.82		
		Cu^{2+}	0.81
Mg^{2+}	0.80		

A scheme was described in Section 2.2 whereby cations present in the Y group were transferred to the X group in the sequence $Li^{+} > Mn^{2+} \gg Fe^{2+} > Co^{2+} > Mg^{2+}$. From charge and ionic radius

considerations this scheme has been extended to include Zn^{2+} and Cu^{2+} viz.

$$Li^{+} > Mn^{2+} \gg Fe^{2+} > Co^{2+} \geq Zn^{2+} \geqslant Cu^{2+} \geqslant Mg^{2+}$$

The position of Zn^{2+} as one of the last cations to be transferred from the Y to the X group is consistent with the reported occurrence of Zn^{2+} in the Y group of a zinc manganese cummingtonite (Hawthorne & Grundy 1973c).

Lastly the A site, when occupied, accepts large ions such as K^{+}, Na^{+}, Pb^{2+}. Ca^{2+}, Ba^{2+}, and Sr^{2+} may be considered together as possible occupants. Phillips (1963) has further suggested that H^{+} (protons) may occupy the A site under exceptional circumstances.

2.4. MINDATA5: A computer program incorporating the derived allocation scheme.

The allocation scheme described in the previous sections has been incorporated into a computer program entitled MINDATA5. The program, written in PL/1, is a modified version of R. Phillips' MINDATA3 in which the allocation scheme has been amended, lengthened and the arithmetic base altered to floating point arithmetic. A listing of the program including operating instructions is given in Appendix 4. A brief summary of the program logic giving the complete form of the allocation scheme is included below.

1) and 2) as MINDATA3, (see page 17).

3) Allocate all Si^{4+}, Be^{2+} and B^{3+} to the Z group and make up to a total of 8.0 atoms with Al^{3+}. Any remaining Al^{3+} is transferred to the Y group. Errors are raised if either Si^{4+}, or $Si^{4+} + Be^{2+}$

or $Si^{4+} + Be^{2+} + B^{3+}$ exceeds 8.08 atoms or $Si^{4+} + Be^{2+} + B^{3+} + Al^{3+}$ is less than 7.95 atoms. A warning is printed if phosphorus is present.

4) Initially allocate all Al^{vi}, Ti^{4+}, Zr^{4+}, Cr^{3+}, V^{3+}, Fe^{3+}, Li^{+}, Ni^{2+}, Co^{2+}, Zn^{2+}, Mg^{2+}, Cu^{2+}, Fe^{2+}, Mn^{2+} to the Y group and sum the total number of cations. If the sum exceeds 5.05, cations are transferred to the X group in the order Li^{+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Zn^{2+}, Cu^{2+}, Mg^{2+} until the Y group total is lowered to 5.0.

5) As MINDATA3.

6) In the unlikely event that the X group total exceeds 2.0 atoms ($\sum Y > 7.0$) all Ca^{2+}, Ba^{2+}, Sr^{2+}, Cd^{2+}, Pb^{2+}, Na^{+}, K^{+}, enters the A group. A test is made to see if the analysis resembles proto-amphibole (Gibbs 1969) by comparing the Li^{+} content in X with the excess of the X group. If Li^{+} exceeds the excess, Li^{+} is transferred to the A group until the X group total is reduced to 2.0.

7) If the sum of the X group is less than 2.0 the group is made up to 2.0 with Ca^{2+}, Ba^{2+}, Sr^{2+}, Pb^{2+}, Cd^{2+}. Any excess of these cations is transferred to the A site in the sequence Cd^{2+}, Ca^{2+}, Ba^{2+}, Sr^{2+}, Pb^{2+}. All Na^{+}, K^{+} enters the A group.

8) Lastly, if the X group total including Ca^{2+}, Ba^{2+}, Sr^{2+}, Cd^{2+}, Pb^{2+}, is less than 2.0 the group is completed in the order Na^{+}, K^{+}, any excess entering the A group in the reverse order.

MINDATA5 also calculates a basic atomic formula from the atomic formulae according to the method of Phillips & Layton (1964).

2.5. Evaluation of MINDATA5.

The four measures Sa, Sb, Sc, and Sd were calculated from the results of MINDATA5 for all the analyses in Appendix 3. As might

be expected, since MINDATA5 was written in the light of the experimentally determined cation distributions histograms of measures Sb (Fig. 2.1) and Sd (Fig. 2.2) show a higher proportion of analyses close to zero than obtained using MINDATA3. Only three analyses, a cummingtonite (27) and two tremolites (43,53) (see Appendix 3) have discrepancies of either Sb or Sd in excess of 0.5. A check was made to see if values for Sb and Sd were consistently lower than those for the same analyses using MINDATA3. With the exception of seven analyses this was found to be the case.

Statistics for measures Ss and Sc are given in Tables 2.4, 2.5. Values for the statistics are all close to zero indicating in general an excellent agreement between experimentally determined and calculated group populations. A comparison with the same statistics calculated using MINDATA3 (Tables 2.1, 2.2) shows a considerable improvement. This applies in particular to Fe^{2+}, Mn^{2+}, Mg^{2+} and Li^{+}. A comparison of the variances (σ^2) of measures Ss and Sc for Fe^{2+}, Mn^{2+}, Mg^{2+}, Li^{+} using the F variance ratio test, demonstrated that the reduction in variance between MINDATA3 and MINDATA5 was statistically significant at the 1 per cent level for Mn^{2+}, Mg^{2+} and at the 5 per cent level for Fe^{2+} and Li^{+}. The remaining cations are essentially unaffected by modifications to the allocation scheme and so too are their respective measures.

In detail there remain minor discrepancies between the experimentally determined and calculated group populations. These are not wholly unexpected considering the simplifying assumptions which were made in deriving the allocation scheme (Section 2.2). However, in Fig. 2.1d, no fewer than 79 per cent of analyses show a mean absolute difference between the calculated and experimentally determined group population of less than 0.2 atoms and 91 per cent less than 0.3 atoms (73 and 91 per cent to 24(O) respectively, Fig. 2.1b).

Table 2.4. Statistics of measure Sa calculated using MINDATA5

Cation	Group	24(O) $\bar{x}$	24(O) σ	24(O) $\lvert\bar{x}\rvert$	24(O) n	23(O) $\bar{x}$	23(O) σ	23(O) $\lvert\bar{x}\rvert$	23(O) n
Si^{4+}	Z	-0.003	0.065	0.054	9	-0.060	0.100	0.069	9
Al^{3+}	Z	-0.021	0.054	0.047	7	0.061	0.119	0.070	7
Be^{2+}	Z	0.010	-	0.010	1	0.010	-	0.010	1
Ti^{4+}	Y	0.037	0.074	0.043	7	0.028	0.071	0.037	7
Al^{3+}	Y	-0.020	0.075	0.055	13	-0.083	0.124	0.085	13
Fe^{3+}	Y	0.010	0.144	0.096	22	0.010	0.142	0.092	22
Fe^{2+}	Y	-0.066	0.189	0.140	46	-0.055	0.191	0.139	76
Mn^{2+}	Y	-0.140	-	0.140	1	-0.200	-	0.200	1
Mg^{2+}	Y	0.045	0.130	0.078	26	0.035	0.162	0.091	27
Co^{2+}	Y	0.180	-	0.180	1	0.180	-	0.180	1
Fe^{2+}	X	0.116	0.199	0.176	24	0.026	0.241	0.172	48
Mn^{2+}	X	0.028	0.053	0.044	5	0.026	0.077	0.046	5
Mg^{2+}	X	-0.111	0.157	0.119	14	-0.144	0.168	0.149	15
Co^{2+}	X	-0.540	-	0.540	1	-0.530	-	0.530	1
Li^{+}	X	0.020	0.030	0.030	2	-0.005	0.025	0.005	2
Ca^{2+}	X	-0.001	0.054	0.029	18	-0.001	0.046	0.027	18
Na^{+}	X	0.007	0.192	0.116	15	0.019	0.165	0.087	15
K^{+}	X	-0.020	-	0.020	1	-0.020	-	0.020	1
Na^{+}	A	-0.038	0.121	0.111	6	-0.057	0.170	0.123	6
K^{+}	A	0.00	0.014	0.01	4	0.005	0.027	0.020	4
Ca^{+}	A	0.010	-	0.010	1	0.010	-	0.010	1
Pb^{+}	A	0.00	-	0.00	1	0.00	-	0.00	1
Li^{+}	A	-0.300	-	0.300	1	-0.020	-	0.020	1

Table 2.5. Statistics of measure Sc calculated using MINDATA5

Cation	Group	24(0) $\bar{x}$	24(0) σ	24(0) $\lvert\bar{x}\rvert$	24(0) n	23(0) $\bar{x}$	23(0) σ	23(0) $\lvert\bar{x}\rvert$	23(0) n
Si^{4+}	Z	0.00	0.00	0.00	8	0.00	0.00	0.00	8
Al^{iv}	Z	0.010	0.096	0.062	11	0.070	0.104	0.79	11
Be^{2+}	Z	0.00	-	0.00	1	0.00	-	0.00	1
Ti^{4+}	Y	0.011	0.028	0.011	7	0.011	0.028	0.011	7
Al^{vi}	Y	-0.074	0.271	0.124	14	-0.127	0.260	0.137	14
Fe^{3+}	Y	0.002	0.010	0.002	21	0.002	0.010	0.002	21
Fe^{2+}	Y	-0.091	0.197	0.117	47	-0.071	0.181	0.100	75
Mn^{2+}	Y	-0.040	-	0.040	1	-0.050	-	0.050	1
Mg^{2+}	Y	0.037	0.092	0.053	25	0.040	0.091	0.053	26
Co^{2+}	Y	0.190	-	0.190	1	0.190	-	0.190	1
Fe^{2+}	X	0.081	0.222	0.148	18	0.017	0.155	0.074	39
Mn^{2+}	X	-0.010	0.043	0.030	4	0.002	0.034	0.022	4
Mg^{2+}	X	-0.061	0.120	0.093	13	-0.077	0.112	0.096	14
Co^{2+}	X	-0.190	-	0.190	1	-0.190	-	0.190	1
Li^{+}	X	-0.040	0.040	0.040	2	-0.025	0.029	0.025	2
Ca^{2+}	X	-0.067	0.228	0.067	18	0.00	0.067	0.00	18
Na^{+}	X	-0.145	0.374	0.208	15	-0.103	0.247	0.135	15
K^{+}	X	0.00	-	0.00	1	0.00	-	0.00	1
Na^{+}	A	-0.070	0.089	0.080	6	-0.073	0.103	0.080	6
K^{+}	A	0.00	0.00	0.00	4	-0.040	0.080	0.040	4
Ca^{+}	A	0.00	-	0.00	1	0.00	-	0.00	1
Pb^{+}	A	0.00	-	0.00	1	0.00	-	0.00	1
Li^{+}	A	0.080	-	0.080	1	0.050	-	0.050	1

It is suggested that for most purposes this is adequate.

In describing the allocation scheme it has been assumed that variation in ordering was dependant upon bulk chemistry alone and was independant of the physical conditions, in particular temperature during crystallisation and subsequent cooling. Various degrees of order - disorder between the M1, M2, and M3 sites of the Y group have been reported. Prentice (1967), Burns & Prentice (1968) and Bancroft & Burns (1969) suggested that magnesioriebeckite from pegmatites showed more disordered Y group cations than crocidolites or glaucophanes from lower temperature metamorphic environments and Litvin et al. (1972) put forward evidence for differences in Fe^{2+}, Fe^{3+}, Al^{3+} Mg^{2+} ordering between the M1, M2, M3 sites of the Y group in 'hornblendes' from the amphibolite and granulite facies. Moreover, Mossbauer studies of cummingtonite (Ghose & Weidner 1972) and anthophyllite (Seifert & Virgo 1974), heated under controlled oxygen fugacities have demonstrated the temperature and time dependance of the Mg^{2+} - Fe^{2+} distribution between the X (M^4) and Y (M1, M2, M3) groups for such amphiboles. These latter findings are of particular importance in the present context since it indicates variation of order - disorder between groups of sites.

Site populations for the three unheated cummingtonites investigated by Ghose & Weidner (1972) and the anthophyllite studied by Seifert & Virgo (1974) are included in Appendix 3 (specimens 9, 38, 39 and 3 respectively). Values for the measure Sb and Sd for both the unheated and heated amphiboles are given in Table 2.6. The difference between the values for Sb and Sd for the unheated amphiboles and those for the heated samples is a measure of the additional variation in ordering introduced by heating and preserved by subsequent quenching under experimental conditions. Compared with the observed discrepancies in Sb and Sd obtained from the results of MINDATA5 the

Table 2.6. Measures Sb and Sd for experimentally heated cummingtonite and anthophyllite.

Cummingtonite (Ghose & Weidner 1972)

No.	Measure	Unheated	390°C	500°C	600°C	700°C
9	Sb	0.490		0.575	0.590	0.670
9	Sd	0.115		0.133	0.143	0.160
38	Sb	0.180			0.375	
38	Sd	0.055			0.155	
39	Sb	0.200	0.210	0.315	0.465	0.520
39	Sd	0.032	0.033	0.071	0.100	0.113

Anthophyllite (Seifert & Virgo 1974)

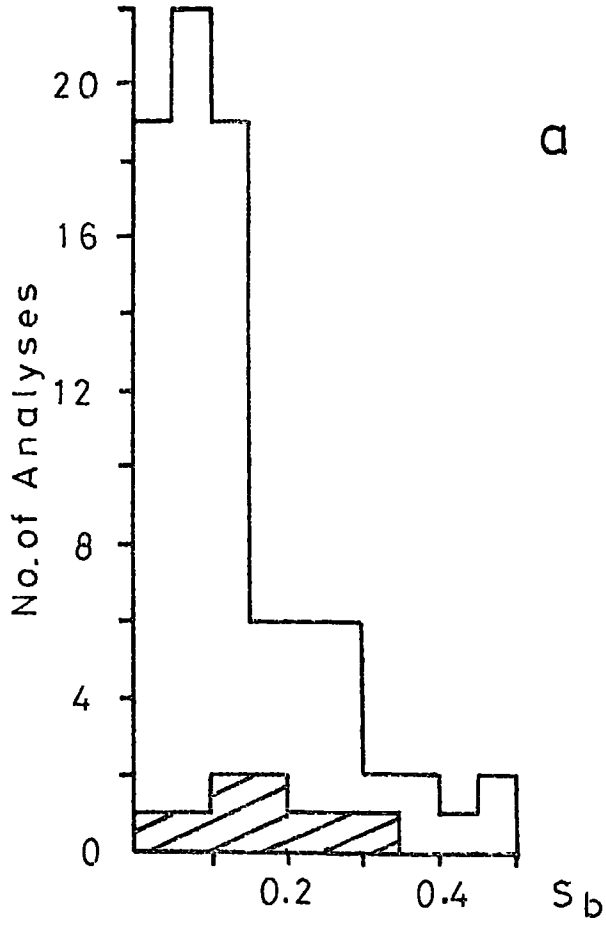
No.	Measure	Unheated	720°C
3	Sb	0.105	0.370
3	Sd	0.040	0.160

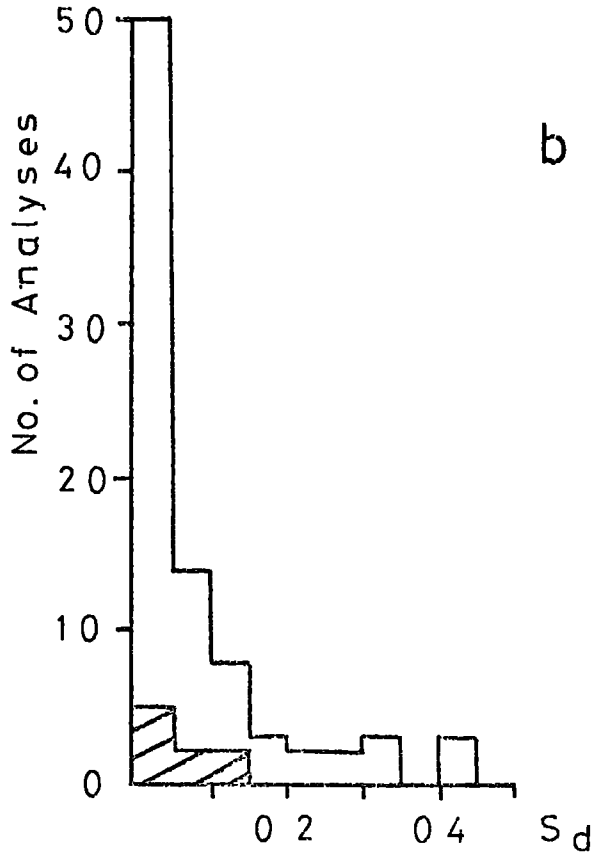
additional variation is of a similar magnitude, see Fig. 2.4., and if present in natural amphiboles would act as a limit to further refinement of MINDAT15 using bulk chemistry alone. However, both Ghose & Weidner (1972) and Seifert & Virgo (1974) have found that at temperatures above approximately 425°C for cummingtonite and 270°C for anthophyllite the rate of cation exchange between the X and Y groups is large compared with the rate of cooling under geological conditions. Since, with one exception, the heating experiments were performed above these temperatures it is to be expected that variation in ordering due to the cooling history of natural amphiboles will be less pronounced than in the quenched amphiboles. In this connection it is of interest to note that Buckley & Wilkins (1971) found no difference in the ordering of Fe^{2+} between the X and Y groups of a cummingtonite in a rhyolitic pumice breccia and a metamorphic cummingtonite, and Wilkins (1970) could find no systematic difference in the Mg^{2+}, Fe^{2+} ordering between the M1, M2 and M3 sites in tremolite - actinolites from greenschist and amphibolite facies. It is tentatively suggested that thermally induced ordering between groups of sites in natural amphiboles is relatively minor compared with the remaining discrepancies between experimentally determined and calculated site populations.

Fig. 2.4. Variation of the measures Sb and Sd due to thermally induced order - disorder.

(a) Variation in Sb produced by thermally induced order - disorder (hatched) compared with the residual discrepancies between experimentally determined cation distributions and those calculated using MINDATA5, 23(0), data from Fig. 2.1d.

(b) Variation in Sd, as above, data from Fig. 2.2d.


a
No. of Analyses
20
16
12
8
4
0
0.2
0.4
S_b


b
No. of Analyses
50
40
30
20
10
0
0 2
0 4
S_d

3. A METHOD FOR ESTIMATING THE IRON OXIDATION STATE IN AMPHIBOLES USING THE BASIC ATOMIC FORMULA

Mention has been made in Chapter 1 of the difficulties involved in determining the iron oxidation state in the growing number of amphiboles analysed by electron microprobe. A method for making such estimates based on the basic atomic formula of Phillips & Layton (1964) and Phillips (1966) was briefly outlined. In the present Chapter the method is described in detail and evaluated using simple theoretical analyses with known oxidation state, (Section 3.1) and published 'real' analyses of known oxidation state (Section 3.2).

The use of the basic atomic formula in the estimation of the iron oxidation state assumes that:-

1) The remaining cations have been determined accurately.
2) The analysis is of a calciferous or alkali amphibole in the sense of Phillips (1966). Oxyamphiboles are excluded.
3) The basic atomic formula condition $(Na^A + Al^Y) = (Na^X + Al^Z)$ holds for amphiboles in which the iron oxidation state has been determined. An examination of a considerable number of basic atomic formulae of published analyses of amphiboles (Chapter 6) shows this to be the case.

3.1. Theoretical analyses of known oxidation state.

In order to evaluate the method, estimates of the iron oxidation state were made for a number of theoretical amphibole atomic formulae of known iron oxidation state, see Table 3.1. For each of the atomic formulae $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$. It should be noted that these atomic formulae, while falling within amphibole compositional space (Phillips 1966), do not necessarily correspond to known amphiboles. For simplicity, all the formulae

Table 3.1. Atomic formulae and nomenclature, after Phillips (1966), of theoretical compositions used to evaluate the basic atomic formula estimate of iron oxidation state.

Number	Atomic formula	Basic formula
1	$\square Na^{+}_{2} Fe^{2+}_{3} Fe^{3+}_{2} Si^{4+}_{8} O^{2-}_{22} (OH)_{2}$	G
2	$Na^{+} Na^{+}_{2} Mg^{2+}_{2} Fe^{2+}_{2} Fe^{3+} Si^{4+}_{8} O^{2-}_{22}(OH^{-})_{2}$	Ec
3	$\square Na^{+}_{2} Fe^{2+}_{3} Fe^{3+} Al^{3+} Si^{4+}_{8} O^{2-}_{22} (OH^{-})_{2}$	G
4	$Na^{+} Ca^{2+} Na^{+} Fe^{2+}_{5} Si^{4+}_{8} O^{2-}_{22} (OH^{-})_{2}$	R
5	$Na^{+}Ca^{2+}Na^{+} Fe^{2+}_{4} Fe^{3+} Si^{4+}_{7} Al^{3+} O^{2-}_{22} (OH^{-})_{2}$	$R_{50}Su_{50}$
6	$Na^{+}Ca^{2+}_{2} Mg^{2+}_{3} Fe^{2+} Fe^{3+} Si^{4+}_{6} Al^{3+}_{2} O^{2-}_{22} (OH^{-})_{2}$	Pa
7	$\square Ca^{2+}_{2} Mg^{2+} Fe^{2+}_{2} Fe^{3+}_{2} Si^{4+}_{6} Al^{3+}_{6} O^{2-}_{22} (OH^{-})_{2}$	Ts
8	$Na^{+} Na^{+}_{2} Fe^{2+}_{3} Fe^{3+}_{2} Si^{4+}_{7} Al^{3+} O^{2-}_{22} (OH^{-})_{2}$	M
9	$\square Ca^{2+}_{2} Fe^{2+}_{3} Fe^{3+} Al^{3+} Si^{4+}_{6} Al^{3+}_{2} O^{2-}_{22} (OH^{-})_{2}$	Ts
10	$\square Na^{+} Ca^{2+} Fe^{2+}_{3} Fe^{3+} Al^{3+} Si^{4+}_{7} Al^{3+} O^{2-}_{22} (OH^{-})_{2}$	$Ts_{50}G_{50}$
11	$Na^{+} Ca^{2+}_{0.2} Na^{+}_{1.8} Fe^{2+}_{4.2} Fe^{3+}_{0.4} Al^{3+}_{0.4} Si^{4+}_{8} O^{2-}_{22} (OH^{-})_{2}$	$Ec_{80}R_{20}$
12	$Na^{+}_{0.5} Ca^{2+}_{1.5} Na^{+}_{0.5} Mg^{2+}_{2} Fe^{2+} Fe^{3+} Al^{3+} Si^{4+}_{6} Al^{3+}_{2} O^{2-}_{22} (OH^{-})_{2}$	$Ts_{50}Su_{50}$
13	$Na^{+} Na^{+}_{2} Fe^{2+}_{3} Fe^{3+}_{0.5} Al^{3+}_{1.5} Si^{4+}_{7} Al^{3+} O^{2-}_{22} (OH^{-})_{2}$	M
14	$Na^{+} Ca^{2+}_{2} Mg^{2+}_{2} Fe^{2+}_{2} Fe^{3+}_{0.25} Al^{3+}_{0.75} Si^{4+}_{6} Al^{3+}_{2} O^{2-}_{22} (OH^{-})_{2}$	Pa

are Li^{+}, Ti^{4+} free and no Y group vacancies occur. Atomic formulae with these features will be considered in Section 3.1.4.

Each atomic formula was converted to weight per cent of the constituent oxides. To simulate an electron microprobe analysis all iron was converted to equivalent FeO and water was neglected. Basic atomic formulae were calculated using MINDAT45 at various $Fe^{2+}/(Fe^{2+} + Fe^{3+})$ ratios, with total iron remaining constant. The ratio $Fe^{2+}/(Fe^{2+} + Fe^{3+})$ is here referred to as the 'reduced iron ratio' and is related to the more common 'iron oxidation state' by the relationship

reduced iron ratio = 1 - iron oxidation state.

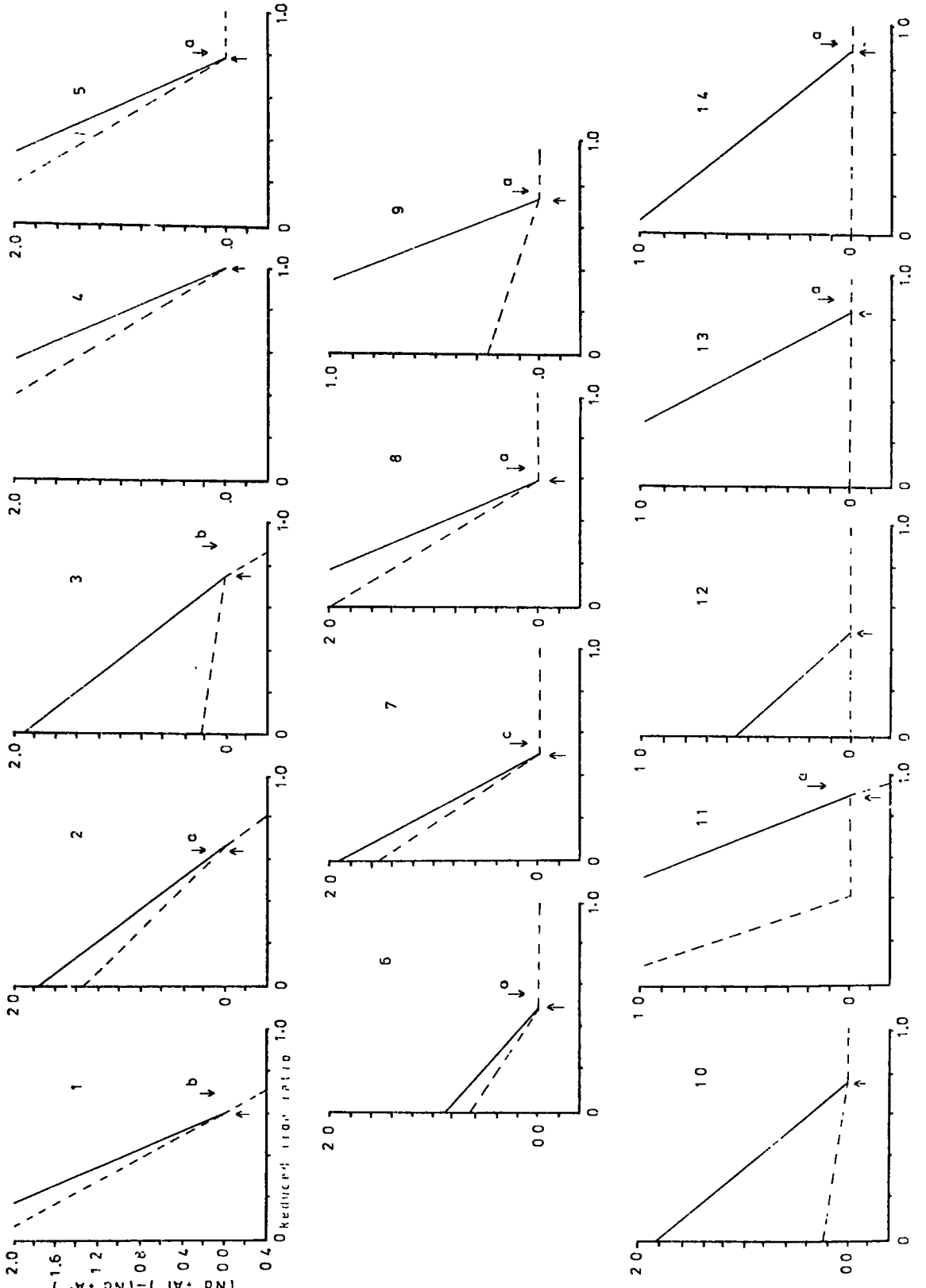
The reduced iron ratio was defined in this way in order that the value of the ratio increased as the Fe^{2+} component and the numerical value of the cations increased (for details see Section 3.1.2.). Plots of the value $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$, with reduced iron ratio for theoretical atomic formulae are given in Fig. 3.1 (dashed line). The actual oxidation state is included for comparison.

Examination of Fig. 3.1. (dashed line) reveals three types of analyses, (i) those for which a unique reduced iron ratio is indicated, viz. 1 to 4, (ii) those for which a limited range of reduced iron ratios are possible, viz. 5 to 11, and (iii) those for which all reduced iron ratios are possible, viz. 12 to 14. As a means of estimating the iron oxidation state of analyses of the third type the basic atomic formula, at least in its simplest sense, is not directly applicable. The significance of the solid curves in Fig. 3.1. is discussed below.

At first sight the existence of analyses which yield $(Na^{A} + Al^{Y})$ equal to $(Na^{X} + Al^{Z})$ for all reduced iron ratios appears to be something of an anomaly. However, a more detailed examination of

Fig. 3.1. Plots of the variation of basic atomic formula $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ with reduced iron ratio for the theoretical atomic formulae listed in Table 3.1.

The dashed line indicates the variation of $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ directly, while the solid line shows the variation assuming that the substitution $2R^{3+} + \square = 3R^{2+}$ is inappropriate. Upward pointing arrows indicate the actual iron oxidation state (as a reduced iron ratio) and downward pointing arrows the lowest reduced iron ratio at which one, or more, of the following constraints are violated, (a) $Na^{A} \leqslant 1.01$, (b) $Si \leqslant 8.08$, (c) $Ca \leqslant 2.02$.


1
2
3
4
5
6
7
8
9
10
11
12
13
14
a
b
c
d
2.0
1.0
0

the method used to calculate the basic atomic formula and the allocation scheme of ions indicates that a similar situation holds for the majority of amphibole analyses. At the same time it is possible to demonstrate that the differing types of plots observed in Fig. 3.1 are not haphazard but are related to the location of the analysis in amphibole compositional space. In Section 3.1.1 the derivation of the basic atomic formula is described in greater detail and in Section 3.1.2 a notation is developed to describe the variation in the basic atomic formula with reduced iron ratio. In Section 3.1.3 the extent of the reduced iron ratio over which $(Na^A + Al^Y) = (Na^X + Al^Z)$ is outlined in terms of bulk chemistry. The method is extended in Section 3.1.4 to theoretical compositions with Li^+, Ti^{4+} and Y group vacancies and in Section 3.1.5 the method is evaluated.

3.1.1. The basic atomic formula.

The basic atomic formula may be written as

$$Na^A\ (Ca\ Na^X)_2\ (Mg\ Al^Y)_5\ (Si\ Al^Z)_8\ O_{22}\ (OH)_2$$

where

$Al^Z = M^{3+} + 2M^{2+}$ in Z,

$Si = Si^{4+}$,

$Al^Y = M^{3+} + 2M^{4+}$ in Y, (excluding any M^{3+}, M^{4+} included in Mg, see below).

$Mg = M^{2+}$ in Y plus any charge balancing substitutions of the type

$Al^{3+} + Li^+ = 2Mg^{2+}$, $\quad Fe^{3+} + Li^+ = 2Mg^{2+}$,

$Ti^{4+} + \square = 2Mg^{2+}$, $\quad 2R^{3+} + \square = 3R^{2+}$,

$Fe^{3+} + O^{2-} = Fe^{2+} + OH^-$,

$Na^X = M^+$ in X,

$Ca = M^{2+}$ in X,

$Na^A = M^+ + 2M^{2+}$ in A.

Excluding the oxyamphiboles, ferric iron enters Al^{Y} unless Li^{+} is present, or there are Y group vacancies. Ferrous iron is included in Mg unless the sum of the Y group exceeds 5.05, (see Chapter 2), in which case Fe^{2+} may be transferred to the X group and included with Ca. When this has occurred the amphibole has moved out of amphibole compositional space. It should be noted that the concepts of the basic atomic formula and amphibole compositional space were originally devised for calciferous and alkali amphiboles. Here, the former concept is implicitly extended to cover compositions in which excess Mn^{2+}, Fe^{2+}, Mg^{2+} etc. from Y may enter the X group.

3.1.2. Variation of the components of the basic atomic formula with reduced iron ratio.

By calculating an atomic formula from a chemical analysis using the 23(O) anion base the sum of the positive charges is constant at 46. The change from Fe_2O_3 to FeO rich compositions (weight per cent of all remaining oxides constant) must correspond to an increase in the number of all the other cations present. The increase is dependant on the amount of each cation already present and is designated here by Δ. In the following discussion it is not necessary to know the numerical value of Δ. To maintain a constant total charge of 46+ the decrease in charge associated with the conversion of Fe^{3+} to Fe^{2+} is equal to the sum of the increments (Δ) of the remaining cations multiplied by their charge. Using the basic atomic formula rather than individual cations, to maintain charge neutrality the change in charge associated with a change in the amount of Fe^{3+} by Δ is given by:-

$$3\Delta Fe^{3+} = -\Delta Na^{A} - 2\Delta Ca - \Delta Na^{X} - 2\Delta Mg - 3\Delta Al^{Y} - 4\Delta Si - 3\Delta Al^{Z},$$

and the associated change in the amount of Fe^{3+} is

$$Fe^{3+} = -\tfrac{1}{3}\Delta Na^{A} - \tfrac{2}{3}\Delta Ca - \tfrac{1}{3}\Delta Na^{X} - \tfrac{2}{3}\Delta Mg - \Delta Al^{Y} - \tfrac{4}{3}\Delta Si - \Delta Al^{Z}.$$

As the numerical values for the cations increase from low to high reduced iron ratios the allocation of cations also varies. A detailed description of the allocation scheme has been given in Chapter 2. As a convention the change in the amount of an ion, Δ., is taken as an unsigned number. An increase or decrease in the amount of an ion is indicated by a positive or negative sign respectively. Thus $\Delta 1 + \Delta 2 - \Delta 3$ means that the total change in the components is the sum of the increases of 1 and 2 minus the decrease in 3 by their respective delta values.

For convenience basic atomic formula Al^{Y} has been split into a component due to ferric iron alone, $Fe^{3+'}$ and the remaining contribution $Al^{Y'}$, ($Al^{Y} = Al^{Y'} + Fe^{3+'}$). The following changes occur as Fe_2O_3 is converted to FeO, (i.e. low to high reduced iron ratios).

<u>Si</u> $Si = +\Delta Si$,

<u>Al^{Z}</u> (i) $\sum Al^{3+} + Si^{4+} < 8.0$,

$Al^{Z} = +\Delta Al^{Z}$.

(ii) $\sum Al^{3+} + Si^{4+} > 8.0$, $Si^{4+} < 8.0$, (transfer of Al^{Z} to Al^{Y})

$Al^{Z} = -\Delta Si$.

(iii) $Si > 8.0$,

$Al^{Z} = 0.0$.

<u>$Al^{Y'}$</u> (i) $\sum Al^{3+} + Si^{4+} > 8.0$, $Si^{4+} < 8.0$, (transfer of Al^{Z} to Al^{Y})

$Al^{Y'} = +\Delta Al^{Y'} + \Delta Al^{Z} + \Delta Si$.

(ii) $\sum Al^{3+} + Si^{4+} > 8.0$, $Si^{4+} > 8.0$,

$Al^{Y'} = +\Delta Al^{Y'}$.

<u>$Fe^{3+'}$</u> (i) $\sum$ Y + Z groups > 13, no Y group vacancies,

$Fe^{3+'} = \frac{1}{3}\Delta Na^{A} - \frac{1}{3}\Delta Ca - \frac{1}{3}\Delta Na^{X} - \Delta\frac{2}{3}$ Mg $- \Delta Al^{Y'} - \frac{4}{3}\Delta Si - \Delta Al^{Z}$.

(ii) $\sum$ Y + Z groups < 13, Y group vacancies.

An amount of Fe^{3+} equal to twice the number of Y group vacancies is converted to equivalent Mg by the substitution $2R^{2+} + \square = 3R^{2+}$.

Introducing the term Al^{Yo} to signify the appropriate change in $Al^{Y'}$ (see above) and remembering that the change in the number of Y group vacancies depends on changes in the amount of Mg, Al^{Yo} and Fe^{3+}, the change in the amount of ferric iron involved in the above substitution is given by

1) ... $\quad -2\Delta Fe^{3+} + 2\Delta Mg + 2\Delta Al^{Yo}$.

The change in Fe^{3+} is therefore the change in the total amount of Fe^{3+} plus the Fe^{3+} no longer required to balance Y group vacancies

$Fe^{3+'} = -\Delta Fe^{3+} + (-2\Delta Fe^{3+} + 2\Delta Mg + 2\Delta Al^{Yo})$,

2) ... $\quad = -3\Delta Fe^{3+} + 2\Delta Mg + 2\Delta Al^{Yo}$.

Considering a numerical example of an amphibole with $Fe^{3+} = 2.0$, $Mg = 1.6$, $Al^{Yo} = 0.8$, 0.6% group vacancies, 1.2 atoms of Fe^{3+} balancing these and therefore $Fe^{3+'}$ equal to $2.0 - 1.2 = 0.8$. If Mg and Al^{Yo} increase by 0.6 and 0.5 respectively and Fe^{3+} decreases by 0.8 the number of vacancies reduce to 0.3, the amount of ferric iron required to compensate for these is 0.6 and $Fe^{3+'}$ is now $1.2 - 0.6 = 0.6$. The change in the amount of ferric iron required to compensate for the vacancies is therefore 1.2 - 0.6 which is equivalent to an increase in $Fe^{3+'}$ by 0.6. The same result is achieved by substitution in (1).

$$-2 \times 0.8 + 2 \times 0.6 + 2 \times 0.5 = 0.6.$$

However because Fe^{3+} has decreased by 0.8 the total change (decrease) in $Fe^{3+'}$ (-0.8 + 0.6) is given by substituting values of Δ in (2),

$$-3 \times 0.8 + 2 \times 0.6 + 2 \times 0.5 = -0.2.$$

Mg (i) $\sum Y + Z$ groups > 13, no Y group vacancies. (transfer of Mg to Ca)

$$Mg = -\Delta Al^{Yo} + \Delta Fe^{3+'}$$

(ii) $\sum Y + Z$ groups < 13, Y group vacancies.

Here again the substitution $2R^{3+} + \square = 3R^{2+}$ must be considered. For each change in the number of vacancies Mg changes by three times as

much. The change (decrease) in Mg associated with the change in vacancies is given by

$$-3\Delta Fe^{3+} + 3\Delta Mg + 3\Delta Al^{Yo}$$

and the change in Mg as a whole is the difference

$$Mg = \Delta Mg - (-3\Delta Fe^{3+} + 3\Delta Mg + 3\Delta Al^{Yo})$$
$$= +3\Delta Fe^{3+} - 2\Delta Mg - 3\Delta Al^{Yo}$$

Ca i) $\sum Y + Z$ groups < 13.

$$Ca = +\Delta Ca$$

ii) $\sum Y + Z$ groups > 13. (transfer of Mg to Ca)

$$Ca = +\Delta Ca + \Delta Mg + \Delta Al^{Yo} - \Delta Fe^{3+}$$

Na^X i) $\sum Y + Z < 13$, $\sum Ca^{2+} + Na^{+} < 2.0$.

$$Na^X = +\Delta Na^X$$

ii) $\sum Y + Z < 13$, $\sum Ca^{2+} + Na^{+} > 2.0$. (transfer of Na^X to Na^A)

$$Na^X = -\Delta Ca$$

iii) $\sum Y + Z > 13$, $\sum Ca^{2+} + Na^{+} > 2.0$. (transfer of Na^X to Na^A increased by transfer of Mg to Ca).

$$Na^X = -\Delta Ca - \Delta Mg - \Delta Al^{Yo} + \Delta Fe^{3+}$$

iv) $\sum Y + Z > 13$, $\sum Ca^{2+} + Na^{+} < 2.0$.

$$Na^X = +\Delta Na^X$$

Na^A i) $\sum Y + Z < 13$, $\sum Ca^{2+} + Na^{+} > 2.0$. (transfer of Na^X to Na^A)

$$Na^A = +\Delta Na^A + \Delta Na^X + \Delta Ca.$$

ii) $\sum Y + Z > 13$, $\sum Ca^{2+} + Na^{+} > 2.0$, $Ca^{2+} < 2.0$, (transfer of Na^X to Na^A increased by transfer of Mg to Ca)

$$Na^A = +\Delta Na^A + \Delta Na^X + \Delta Ca + \Delta Mg + \Delta Al^{Yo} - \Delta Fe^{3+}$$

iii) $\sum Y + Z > 13$, $\sum Ca^{2+} + Na^{+} > 2.0$, $Ca^{2+} > 2.0$, (transfer of Na^X to Na^A increased by transfer of Mg to Ca)

$$Na^A = +\Delta Na^A + 2\Delta Ca + 2\Delta Mg + 2\Delta Al^{Yo} - 2\Delta Fe^{3+}$$

The factor 2 is introduced because divalent cations are entering the A group.

3.1.3. Variation of the range of reduced iron ratios for which ($Na^A + Al^Y$) equals ($Na^X + Al^Z$) with bulk chemistry.

Knowing how the components of the basic atomic formula vary with the reduced iron ratio it is possible to explain the differences in the results for the various theoretical compositions noted in Fig. 3.1. The explanation which follows is strictly only applicable to theoretical Li^+, Ti^{4+} free amphiboles but the resulting generalisations may be extended to theoretical Li^+, Ti^{4+} amphiboles and actual amphiboles and are discussed in Sections 3.1.4 and 3.2 respectively.

The range of reduced iron ratios over which ($Na^A + Al^Y$) equals ($Na^X + Al^Z$) will be outlined for each of the following general amphibole compositions in turn.

$Al^Z > 0.0$,	$Al^Y > 0.0$,	$Na^X \geqslant 0.0$,	$Na^A > 0.0$.
$Al^Z > 0.0$,	$Al^Y > 0.0$,	$Na^X \geqslant 0.0$,	$Na^A = 0.0$.
$Al^Z = 0.0$,	$Al^Y > 0.0$,	$Na^X \geqslant 0.0$,	$Na^A > 0.0$.
$Al^Z = 0.0$,	$Al^Y > 0.0$,	$Na^X \geqslant 0.0$,	$Na^A = 0.0$.
$Al^Z \geqslant 0.0$,	$Al^Y = 0.0$,	$Na^X \geqslant 0.0$,	$Na^A > 0.0$.

For illustrative purposes it is convenient to subdivide theoretical compositions into two groups, those with $Al^Y = Al^{Y'} + Fe^{3+'}$ and those with $Al^Y = Fe^{3+'}$ at the 'correct' reduced iron ratio.

Starting with a consideration of analyses where $Al^Y = Al^{Y'} + Fe^{3+'}$. For a general composition with $Al^Z > 0.0$, $Al^Y > 0.0$, $Na^X \geqslant 0.0$, $Na^A > 0.0$, such as $Na^+(Na^+ Ca^{2+})_2(Mg^{2+} Fe^{2+} Fe^{3+} Al^{3+})_5 (Si^{4+} Al^{3+})_8 O^{2-}_{22}(OH^-)_2$, ($Na^A + Al^Y$) equals ($Na^X + Al^Z$) for all reduced iron ratios. At low reduced iron ratios the rate of change of ($Na^A + Al^Y$) is the same as that for ($Na^X + Al^Z$), see equation (3).

(3) ----

$Na^A = + \Delta Na^A + \Delta Ca + \Delta Na^X$

$Al^{Y'} = + \Delta Al^{Y'} + \Delta Si + \Delta Al^Z$

$* Fe^{3+'} = -\Delta Na^A - 2\Delta Ca - \Delta Na^X - 2\Delta Mg - 3\Delta Al^{Y'} - 4\Delta Si - 3\Delta Al^Z$.

$+ 2\Delta Mg + 2\Delta Al^{Y'} + 2\Delta Si + 2\Delta Al^Z$

$- \Delta Ca - \Delta Si$

$Na^X = -\Delta Ca$

$Al^Z = -\Delta Si$

$-\Delta Ca - \Delta Si$

---

* The value for $Fe^{3+'}$ is derived from $- 3\Delta Fe^{3+} + 2\Delta Mg + 2\Delta Al^{Yo}$, where $\Delta Fe^{3+} = -\frac{1}{3}\Delta Na^A + \frac{2}{3}\Delta Ca + \frac{1}{3}\Delta Na^X$ ..... etc, and $\Delta Al^{Yo} = \Delta Al^{Y'} + \Delta Si + \Delta Al^Z$.

Similarly for high reduced iron ratios in which the sum of the Y group excedes 5.0, both terms change at the same rate, equation (4). This occurs for compositions in which Na^A is equal to, or greater than zero.

(4) ----

$Na^A = + \Delta Na^A + \Delta Ca + \Delta Na^X + \Delta Mg + \Delta Al^{Y'} + \Delta Si + \Delta Al^Z$

$- \frac{1}{3}\Delta Na^A - \frac{2}{3}\Delta Ca - \frac{1}{3}\Delta Na^X - \frac{2}{3}\Delta Mg - \Delta Al^{Y'} - \frac{4}{3}\Delta Si - \Delta Al^Z$

$Al^{Y'} = + \Delta Al^{Y'} + \Delta Si + \Delta Al^Z$

$Fe^{3+'} = - \frac{1}{3}\Delta Na^A - \frac{2}{3}\Delta Ca - \frac{1}{3}\Delta Na^X - \frac{2}{3}\Delta Mg - \Delta Al^{Y'} - \frac{4}{3}\Delta Si - \Delta Al^Z$

$+ \frac{1}{3}\Delta Na^A - \frac{1}{3}\Delta Ca + \frac{1}{3}\Delta Na^X - \frac{1}{3}\Delta Mg - \frac{2}{3}\Delta Si$

$Na^X = - \Delta Ca - \Delta Mg - \Delta Al^{Y'} - \Delta Si - \Delta Al^Z$

$+ \frac{1}{3}\Delta Na^A + \frac{2}{3}\Delta Ca + \frac{1}{3}\Delta Na^X + \frac{2}{3}\Delta Mg + \Delta Al^{Y'} + \frac{4}{3}\Delta Si + \Delta Al^Z$

$Al^Z = - \Delta Si$

$+ \frac{1}{3}\Delta Na^A - \frac{1}{3}\Delta Ca + \frac{1}{3}\Delta Na^X - \frac{1}{3}\Delta Mg - \frac{2}{3}\Delta Si$

From the definition of the theoretical compositions, at the 'correct' reduced iron ratio $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$ and therefore as both sides of the equation are changing at the same rate the condition will hold for all remaining reduced iron ratios, see Fig. 3.1 nos. 12, 13, 14.

Less general compositions with $Al^Z > 0.0$, $Al^Y > 0.0$, $Na^X \geqslant 0.0$ but $Na^A = 0.0$ yield only a limited range of reduced iron ratios. This can be illustrated for a general formula $\square (Ca^{2+}\ Na^{+})_2(Mg^{2+}\ Fe^{2+}\ Fe^{3+}\ Al^{3+})_5(Si^{4+}\ Al^{3+})_8O^{2-}_{22}(OH^-)$. At low reduced iron ratios, with the sum of the Y group less than 5.0, $(Na^A + Al^Y)$ and $(Na^X + Al^Z)$ change at differing rates, see equation (5).

(5) ----

$$
\begin{array}{lr}
Al^{Y'} = & +\Delta Al^{Y'} + \Delta Si + \Delta Al^{Z} \\
Fe^{3+'} = & -2\Delta Ca - \Delta Na^{X} - 2\Delta Mg - 3\Delta Al^{Y'} - 4\Delta Si - 3\Delta Al^{Z} \\
 & \quad + 2\Delta Mg + 2\Delta Al^{Y'} + 2\Delta Si + 2\Delta Al^{Z} \\
\hline
 & -2\Delta Ca - \Delta Na^{X} \qquad\qquad - \Delta Si \\
\hline
\end{array}
$$

$$
\begin{array}{lr}
Na^{X} = & +\Delta Na^{X} \\
Al^{Z} = & \qquad\qquad - \Delta Si \\
\hline
 & +\Delta Na^{X} \qquad\qquad - \Delta Si \\
\hline
\end{array}
$$

However, for high reduced iron ratios as soon as the sum of the Y group exceeds 5.0 (and $\sum Ca^{2+} + Na^{+} > 2.0$ allowing an overflow from the X to A groups) equation (4) applies. Provided $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$ after these transfers have begun it will hold for all instances at higher reduced iron ratios, Fig. 3.1 nos. 9,10.

Considering analyses lying in the plane $Al^Z = 0.0$ with $Al^Y > 0.0$, $Na^X \geqslant 0.0$, $Na^A > 0.0$. These may be included in the formula $Na^{+}\ (Ca^{2+}\ Na^{+})_2(Mg^{2+}\ Fe^{2+}\ Fe^{3+}\ Al^{3+})_5\ Si^{4+}_8O^{2-}_{22}\ (OH^-)_2$. Taking low reduced iron ratios with Si^{4+} less than 8.0, and the sum of the Y group less than 5.0, the rate of change of $(Na^A + Al^Y)$ equals

that of $(Na^X + Al^Z)$ from equation (3). However, for high reduced iron ratios with Si^{4+} in excess of 8.0 and the sum of the Y group in excess of 5.0 this is no longer the case, see equation (6).

(6) ----

$$
\begin{aligned}
Na^A &= + \Delta Na^A + \Delta Ca + \Delta Na^X + \Delta Mg + \Delta Al^{Y'} \\
&\quad - \tfrac{1}{3}\Delta Na^A - \tfrac{2}{3}\Delta Ca - \tfrac{1}{3}\Delta Na^X - \tfrac{2}{3}\Delta Mg - \Delta Al^{Y'} - \tfrac{4}{3}\Delta Si \\
Al^{Y'} &= + \Delta Al^{Y'} \\
Fe^{3+'} &= - \tfrac{1}{3}\Delta Na^A - \tfrac{2}{3}\Delta Ca - \tfrac{1}{3}\Delta Na^X - \tfrac{2}{3}\Delta Mg - \Delta Al^{Y'} - \tfrac{4}{3}\Delta Si \\
&\quad + \tfrac{1}{3}\Delta Na^A - \tfrac{1}{3}\Delta Ca + \tfrac{1}{3}\Delta Na^X - \tfrac{1}{3}\Delta Mg - \tfrac{8}{3}\Delta Si \\
Na^X &= - \Delta Ca - \Delta Mg - \Delta Al^{Y'} \\
&\quad + \tfrac{1}{3}\Delta Na^A + \tfrac{2}{3}\Delta Ca + \tfrac{1}{3}\Delta Na^X + \tfrac{2}{3}\Delta Mg + \Delta AlY' + \tfrac{4}{3}\Delta Si \\
&\quad + \tfrac{1}{3}\Delta Na^A - \tfrac{1}{3}\Delta Ca + \tfrac{1}{3}\Delta Na^X - \tfrac{1}{3}\Delta Mg + \tfrac{4}{3}\Delta Si
\end{aligned}
$$

It is possible to have a limited range of reduced iron ratios for which $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$ but these are at low values, see Fig. 3.1 no. 11.

All analyses of the general type $Al^Z = 0.0$, $Al^Y > 0.0$, $Na^X \geqslant 0.0$, $Na^A = 0.0$, give a unique reduced iron ratio. This comes about for low and high reduced iron ratios, equations (5) and (6) apply respectively, Fig.3.1 no. 3.

Lastly analyses in which $Al^Y = 0.0$ have only one possible reduced iron ratio and that is for $Fe^{2+} / (Fe^{2+} + Fe^{3+}) = 1.0$. In Fig. 3.2a, the region in amphibole compositional space which gives specific regions of reduced iron ratios for analyses with $Al^Y = Al^{Y'} + Fe^{3+'}$ are illustrated.

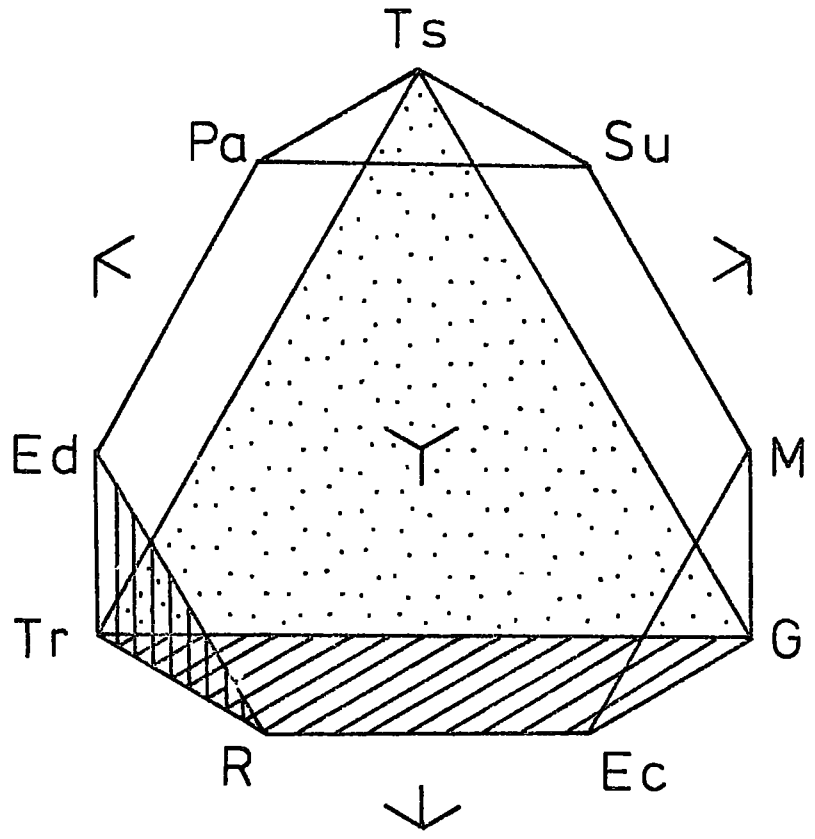
The same approach may be applied to theoretical compositions in which $Al^Y = Fe^{3+'}$ and the resulting extent over which $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$ is given in Fig. 3.2b. $Al^{Y'}$ is absent from low reduced iron ratios and is present only at high reduced iron ratios

Fig. 3.2. Amphibole compositional space showing the extent of reduced iron ratios for which ($Na^A + Al^Y$) equals ($Na^X + Al^Z$).

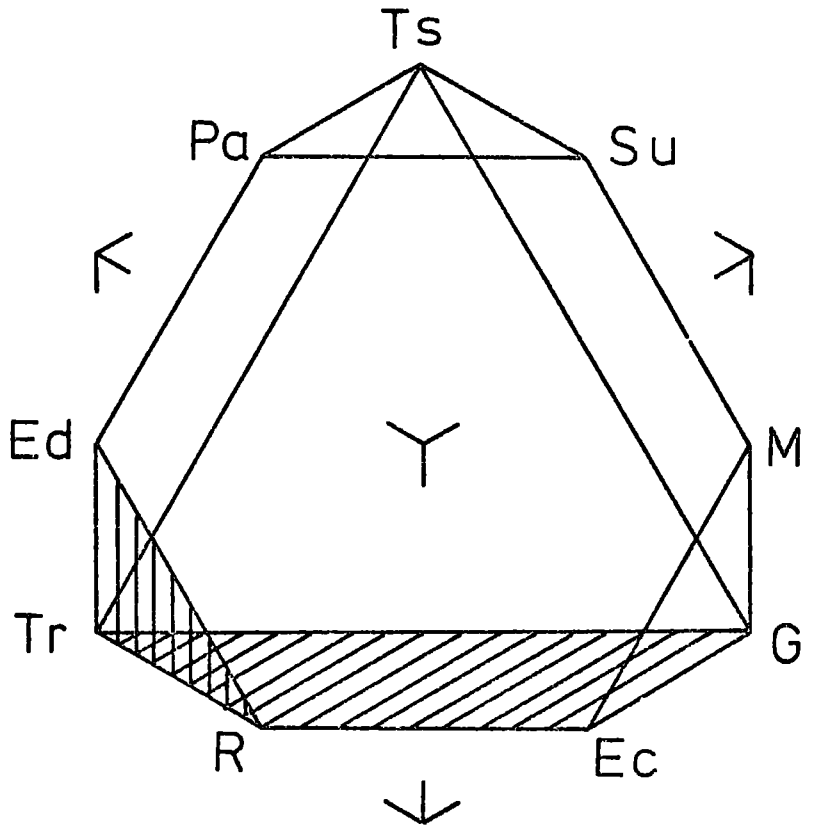
(a) Theoretical compositions in which $Al^Y = Al^{Y'} + Fe^{3+'}$. Unique solutions are found in the plane Tr - Ed - R (vertical shading) and long the join Tr - G. Over the remainder of the plane Tr - R - Ec - G (diagonal shading) a limited range of solutions at low reduced iron ratios are possible. In the plane Tr - Ts - G (dotted) a limited range of solutions are possible at high reduced iron ratios. Elsewhere in amphibole compositional space ($Na^A + Al^Y$) = ($Na^X + Al^Z$) for all reduced iron ratios.

(b) Theoretical compositions in which $Al^Y = Fe^{3+'}$. Regions in which a unique solution is possible are shaded. Throughout the remainder of amphibole compositional space a limited range of reduced iron ratios is possible.

a



b



when $Si^{4+} + Al^{3+}$ is greater than 8.0. This means that for general compositions, only a limited range of reduced iron ratios yield balanced basic atomic formulae Fig.3.1 nos. 5,6,7,8. When there is no Al^{3+} present ($Al^{Z} = 0.0$) a unique solution is possible, see Fig. 3.2b and Fig.3.1 nos. 1,2,4.

It can be seen from the above discussion that the use of the basic atomic formula to estimate the iron oxidation state for theoretical compositions, and by inference actual compositions, will be unsuccessful for the great majority of analyses. The method is likely to be most successful for compositions in which $Al^{Z} = 0.0$, for example riebeckite.

For ferric rich compositions of all these titanium free, theoretical, analyses, the sum of the Y group is less than 5.0. The resultant Y group vacancies are balanced by the substitution $2R^{3+} + \square = 3R^{2+}$. Phillips (1963, p. 709) suggested that this was an uncommon substitution. If instead the substitution is prohibited and the amount of ferric iron involved added to $Fe^{3+'}$ the variation in $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ shown as a solid line in Fig. 3.1 is obtained. The estimated reduced iron ratio is now either a unique value or refers to only a limited range including in every instance the original iron oxidation state. Again it is possible to define the region in amphibole compositional space in which unique or a limited range of solutions will be obtained. Remembering that $Fe^{3+'}$ no longer requires the additional term $-2\Delta Fe^{3+} + 2\Delta Mg + 2\Delta Al^{Yo}$ to account for changes in the number of vacancies in the Y group, it can be seen from equations (3) and (5) that when the sum of the Y group excedes 5.0 both $(Na^{A} + Al^{Y})$ and $(Na^{X} + Al^{Z})$ change at differing rates. The resultant distributions of analyses with $Al^{Y} = Al^{Y'} + Fe^{3+'}$ is the same as that shown in Fig. 3.2b. By making this additional assumption of the inapplicability of the substitution of $2R^{3+} + \square = 3R^{2+}$ it would appear to be possible to

estimate the reduced iron ratio and hence iron oxidation state in a successful manner. The possibility of Y group vacancies associated with titanium ($Ti^{4+} + \square = 2Mg^{2+}$) is not excluded.

In some instances the range of reduced iron ratios may be further constrained by crystal chemical considerations. Three constraints which can be applied are, (i) $Na^{A} \leqslant 1.01$, (ii) $Si \leqslant 8.08$, (iii) $Ca \leqslant 2.02$. It is recognised that (iii) is violated in joesmithite (Moore 1969) but is probably otherwise of general validity (Leake 1968). Where appropriate the lowest reduced iron ratio to violate each of these constraints has been indicated on Fig. 3.1. It can be seen that a combination of the basic atomic formula condition $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z}) = 0.0$, assuming the inappropriateness of the substitution $2R^{3+} + \square = 3R^{2+}$, plus the above crystal chemical constraints allows an accurate reduced iron ratio and hence iron oxidation state to be estimated for theoretical compositions.

3.1.4 Theoretical atomic formulae of known oxidation state with lithium, titanium or Y group vacancies.

All the theoretical compositions considered so far have excluded substitutions of the type $Fe^{3+} + Li^{+} = 2Mg^{2+}$, $Ti^{4+} + \square = 2Mg^{2+}$, or $2R^{3+} + \square = 3R^{2+}$. A number of theoretical atomic formulae with these substitutions are given in Table 3.2. To simulate an electron microprobe analysis all iron was converted to equivalent FeO and water neglected. Plots of the variation of $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ with reduced iron ratio are given in Fig. 3.3. Using the crystal chemical constraints outlined above and assuming that the substitution $2R^{3+} + \square = 3R^{2+}$ is inappropriate estimates of the reduced iron ratio (solid line) can be made satisfactorily for lithium bearing, 15, 16, and titanium bearing analyses, 17, 18, 19.

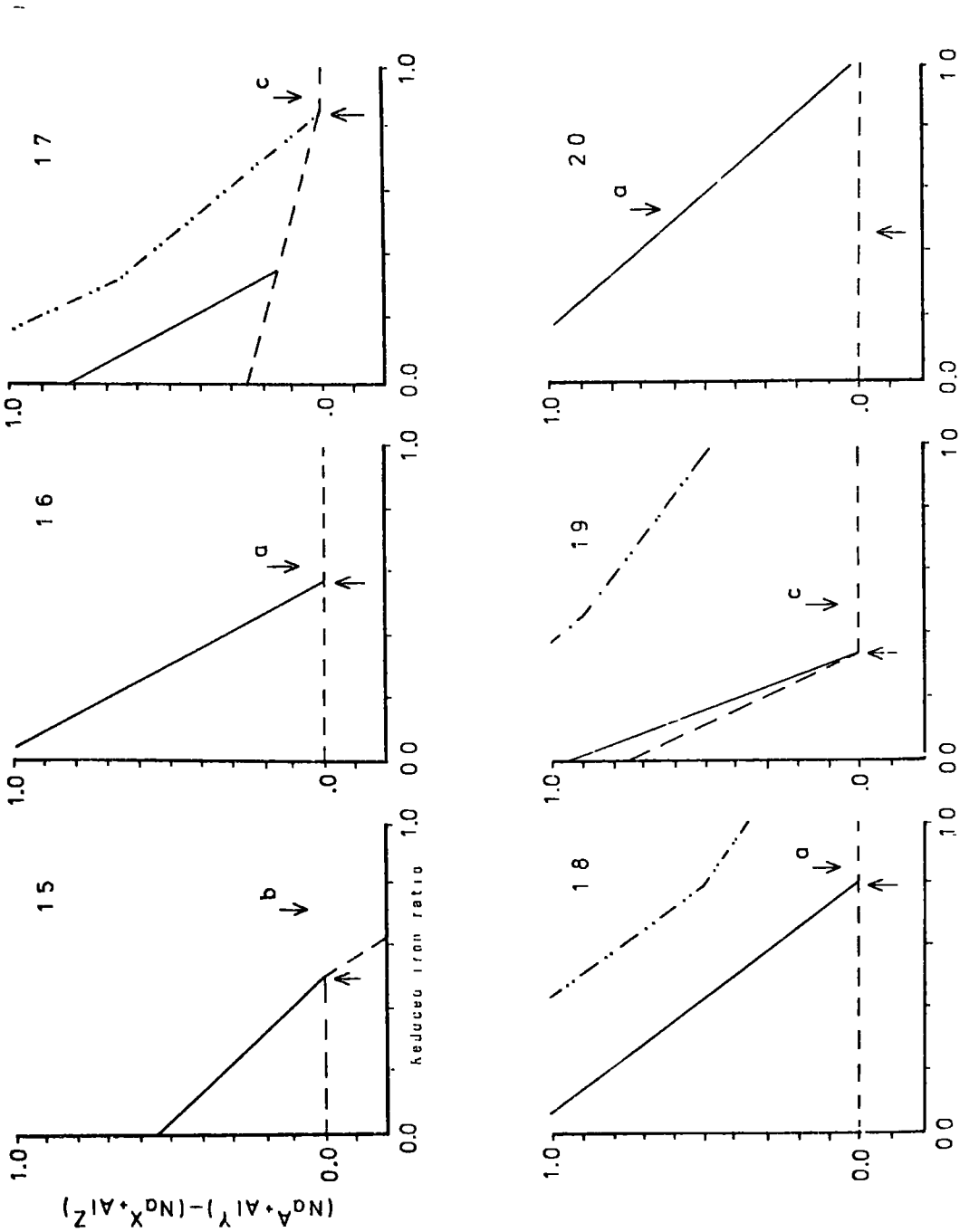
However, that this assumption is incorrect with respect to analysis 20 can be seen because $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ nowhere equals zero (solid line) unless the substitution $2R^{3+} + \square = 3R^{2+}$

Table 3.2. Atomic formulae and nomenclature after Phillips (1966), of theoretical compositions with lithium, titanium, or Y group vacancies.

Number	Atomic formula	Basic formula name
15	$Na^{+}\ Na^{+}_{2}\ Mg^{2+}\ Fe^{2+}\ Fe^{3+}\ Li^{+}\ Al^{3+}\ Si^{4+}_{8}\ O^{2-}_{22}\ (OH^{-})_{2}$	Ec
16	$Na^{+}\ Na^{+}_{2}\ Fe^{2+}_{2}\ Li^{+}_{0.5}\ Fe^{3+}_{1.5}\ Al^{3+}\ Si^{4+}_{7}\ Al^{3+}\ O^{2-}_{22}\ (OH^{-})_{2}$	M
17	$\square Ca^{2+}_{2}\ Mg^{2+}_{0.5}\ Fe^{2+}_{3}\ Fe^{3+}_{0.5}\ Ti^{4+}_{0.5}\ Al^{3+}_{0.5}\ Si^{4+}_{6}\ Al^{3+}_{2}\ O^{2-}_{22}\ (OH^{-})_{2}$	Ts
18	$Na^{+}\ Ca^{2+}_{2}\ Mg^{2+}\ Fe^{2+}\ Fe^{3+}_{0.5}\ Al^{3+}_{0.5}\ Ti^{4+}_{0.5}\ \square_{0.5}\ Si^{4+}_{6}\ Al^{3+}_{2}\ O^{2-}_{22}\ (OH^{-})_{2}$	Pa
19	$\square Ca^{2+}_{2}\ Fe^{2+}\ Fe^{3+}_{2}\ Ti^{4+}\ \square\ Si^{4+}_{6}\ Al^{3+}_{2}\ O^{2-}_{22}\ (OH^{-})_{2}$	Ts
20	$Na^{+}\ Ca^{2+}\ Na^{+}\ Mg^{2+}_{2}\ Fe^{2+}\ Fe^{3+}_{0.5}\ Al^{3+}_{0.5}\ Fe^{3+}_{0.66}\ \square_{0.33}\ Si^{4+}_{7}\ Al^{3+}\ O^{2-}_{22}\ (OH^{-})_{2}$	$R_{50}Su_{50}$

Fig. 3.3. Plots of the variation of basic atomic formula ($Na^A + Al^Y$) - ($Na^X + Al^Z$) with reduced iron ratio for the theoretical atomic formulae listed in Table 3.2.

The identification of the curves is the same as that used in Fig. 3.1, i.e. the broken line indicates the variation in ($Na^A + Al^Y$) - ($Na^X + Al^Z$) directly, the solid line shows the variation assuming that the substitution $2R3^+ + \square = 3R^{2+}$ is inappropriate. In addition for atomic formulae 17 to 19 the curve (-- .. -- .. --) represents the variation of ($Na^A + Al^Y$) - ($Na^X + Al^Z$) assuming that both $2R^{3+} + \square = 3R^{2+}$ and $Ti^{4+} + \square = 2Mg^{2+}$ are inappropriate. Upward pointing arrows indicate the original iron oxidation state and downward pointing arrows the lowest reduced iron ratio at which one, or more, of the following constraints are violated, (a) $Na^A \leqslant 1.01$, (b) $Si^{4+} \leqslant 8.08$ (c) $Ca \leqslant 2.02$.


(NQA+AIY)-(NQX+AIZ)
Reduced iron ratio
15
16
17
18
19
20
a
b
c
1.0
0.0

actually occurs (dashed line).

Just as with ferric iron, titanium when present need not be balancing vacancies in the Y group. However, for ferric rich compositions ($\sum Y < 5.0$) titanium will, if present, be considered as taking part in the substitution $Ti^{4+} + \square = 2Mg^{2+}$, see Chapter 2. This will affect the value for $Al^{Y'}$ and $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$. In Fig. 3.3 a third curve (-- . . -- . . --) is plotted for analyses 17 to 19 assuming that substitutions $2R^{3+} + \square = 3R^{2+}$ and $Ti^{4+} + \square = 2Mg^{2+}$ are both inappropriate. The presence of the substitution $Ti^{4+} + \square = 2Mg^{2+}$ is indicated for analyses 18 and 19 by the failure of $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ to equal zero for any reduced iron ratio.

3.1.5 Comparison of the basic atomic formula and stoichiometric methods for estimating the iron oxidation state of theoretical compositions.

It can be seen from the above discussion that reduced iron ratios can be estimated from the basic atomic formula and, where appropriate by applying crystal chemical constraints plus assumptions concerning the applicability of substitutions involving Y group vacancies. Results obtained for theoretical analyses 1 to 20 by the present method are compared in Table 3.3 and Figs. 3.4, 3.5 with the reduced iron ratios for the same analyses estimated from the four cation bases of Stout (1972), see Chapter 1 for details. The estimated and actual reduced iron ratios are consistent when calculated by the basic atomic formula method, although unless a crystal chemical constraint can be applied to those compositions with $Al^{Y} > 0.0$, $Al^{Z} > 0.0$, or Y group vacancies (nos. 5 to 10, 12 to 20) a range of reduced iron ratios is possible (Table 3.3, and Fig. 3.4). Reduced iron ratios calculated from the four cation bases are not in every case consistent with the original value, see Table 3.3 and Fig. 3.5. The cation base in which the sum of the Y and Z groups is assumed to be 13 ($\sum FM = 13$, Stout 1972) is the most

Table 3.3. Comparison of the actual and calculated reduced iron ratios for the theoretical atomic formula numbers 1 to 20 calculated from basic atomic formula and stoichiometric methods.

mber	Actual reduced iron ratio	Calculated reduced iron ratio (basic atomic formula)	Calculated reduced iron ratio, (cation bases) $\sum$Na=16	$\sum$Na=15	$\sum$Ca=15	$\sum$FM=13
1	0.60	0.60	1.0	0.60	1.0	0.60
2	0.66	0.66	0.66	0.0	1.0	0.66
3	0.75	0.75	1.0	0.75	1.0	0.75
4	1.0	1.0	1.0	0.0	1.0	1.0
5	0.80	0.80-0.83	0.80	0.19	1.0	0.80
6	0.50	0.50-0.52	0.50	0.0	0.50	0.50
7	0.50	0.50-0.56	1.0	0.50	0.50	0.50
8	0.60	0.60-0.66	0.60	0.0	0.50	0.50
9	0.75	0.75-0.78	1.0	0.75	0.75	0.75
0	0.75	0.75-1.0	1.0	0.75	1.0	0.75
1	0.91	0.90	0.90	0.25	1.0	0.90
2	0.50	0.50-1.0	1.0	0.0	1.0	0.50
3	0.85	0.85-0.90	0.85	0.0	1.0	0.85
4	0.89	0.89-0.92	0.89	0.0	0.89	0.89
5	0.50	0.50-0.72	0.50	0.0	1.0	0.50
6	0.57	0.57-0.62	0.57	0.0	1.0	0.57
7	0.86	0.86-0.91	1.0	0.86	0.86	0.86
8	0.80	0.80-0.86	1.0	0.19	1.0	1.0
9	0.33	0.33-0.50	1.0	1.0	1.0	1.0
20	0.46	0.0-0.54	0.91	0.0	1.0	1.0

$\sum$Na=16, cation base of 16 cations, A site full.

$\sum$Na=15, cation base of 15 cations, A site vacant.

$\sum$Ca=15, All cations except Na^+ and presumably K^+ normalised to 15

$\sum$FM=13, All cations normally present in the Y and Z groups normalised to 13.

Fig. 3.4. Comparison of the reduced iron ratio calculated from the basic atomic formula with the actual reduced iron ratio of theoretical amphibole compositions.

The diagonal line corresponds to equal actual and estimated reduced iron ratios. Where two or more analyses have the same actual reduced iron ratio the estimated values have been drawn slightly separated for clarity of representation.

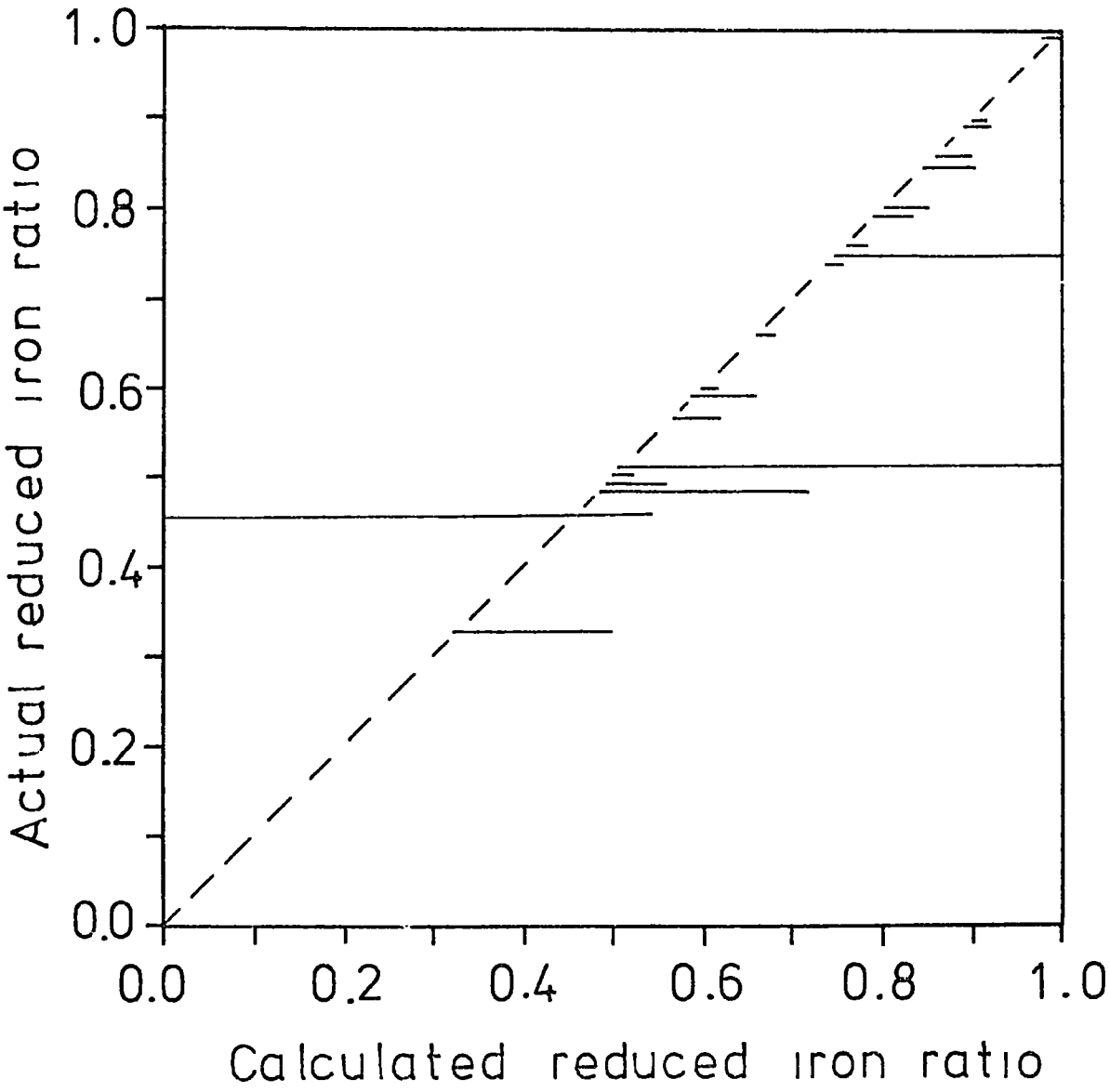

1.0
0.8
0.6
0.4
0.2
0.0
Actual reduced iron ratio
0.0
0.2
0.4
0.6
0.8
1.0
Calculated reduced iron ratio

Fig. 3.5. Comparison of the actual and calculated reduced iron ratios calculated from four cation bases. The nomenclature of the cation bases is taken from Stout (1972).

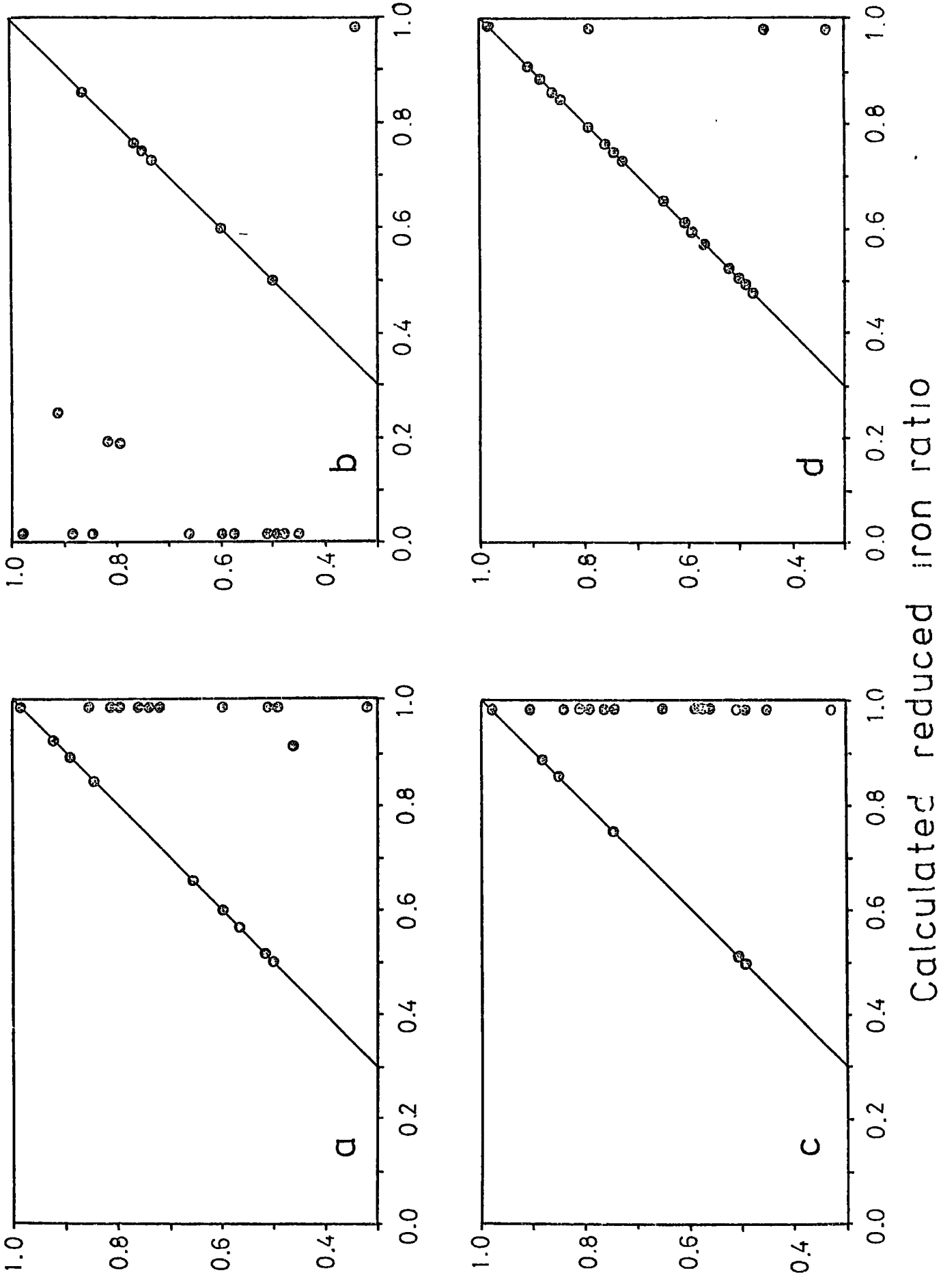
(a) $\sum$ Na = 16, cation base of 16 cations, A site full.

(b) $\sum$ Na = 15, cation base of 15 cations, A site vacant.

(c) $\sum$ Ca = 15, all cations except Na^+ (and presumably K^+) normalised to 15.

(d) $\sum$ FM = 13, all cations normally present in the Y and Z groups normalised to 13.

The diagonal line corresponds to equal actual and estimated reduced iron ratios.


a
b
c
d
Actual reduced iron ratio
Calculated reduced iron ratio
0.0
0.2
0.4
0.6
0.8
1.0

applicable but fails when considering compositions with Y group vacancies such as 18, 19 and 20, Fig. 3.5d.

It is illustrative to compare the relative merits of the cation base $\sum TM = 13$ and the basic atomic formula method. Both indicate the iron oxidation state for calciferous and alkali amphiboles in which the sum of the Y and Z groups is 13, at the actual iron oxidation state. However, for calciferous and alkali amphiboles in which $Al^{Y} > 0.0$, $Al^{Z} > 0.0$, a range of reduced iron ratios is possible with the basic atomic formula method. As mentioned previously this is associated with transfer of cations between components in the basic atomic formula, in particular Mg from Y to Ca in X, as the sum of the Y and Z groups exceeds thirteen. On the other hand the basic atomic formula is applicable to analyses with Y group vacancies while the cation base is not. Both methods are inapplicable to compositions in which the sum of the Y group exceeds five at the actual oxidation state (i.e. for non-calciferous / -alkali amphiboles). In the case of the basic atomic formula a considerable range of iron oxidation states extending from the ratio at which $\sum Y = 5.0$ towards higher reduced iron ratios (lower oxidation states) is to be expected as a result of the transfer of cations between groups.

It is suggested that the basic atomic formula is superior to the use of cation bases in the estimation of the reduced iron ratio and hence iron oxidation state. However, like the cation bases the basic atomic formula method is dependent upon the accuracy of the determination of all the other ions present.

3.2. Real analyses with known iron oxidation state.

In order to evaluate the basic atomic formula method under more realistic circumstances, estimates of the oxidation state were made for a number of published analyses of calciferous and alkali

amphiboles chosen at random from the amphibole data file (Chapter 4). Estimates made in this way were compared with the known actual iron oxidation state, and with estimates made using Stout's cation bases. To avoid using incomplete or inferior analyses the analyses chosen conformed to all the following criteria.

1) Iron oxidation state determined,
(2) $OH^- + F^- + Cl^- + H^+$ calculated from the 24(O) base, in the range 1.8 - 2.2, to exclude oxyamphiboles,
3) Analysis total in the range 99.5 - 100.5 per cent,
4) When calculated to the 23(O) base basic atomic formula $(Na^A + Al^Y) - (Na^X + Al^Z)$ was less than 0.01.

All iron was converted to equivalent FeO and H_2O^+, F, Cl neglected. Estimates of the reduced iron ratio were made for 18 analyses, see Table 3.4. For those analyses in which a complete range of reduced iron ratios was possible it was assumed that the substitution $2R^{3+} + \square = 3R^{2+}$ was inapplicable. The three crystal chemical constraints mentioned in Section 3.1.3 were also applied where appropriate. The results are given in Table 3.4 and Fig 3.6 where they are compared with the actual reduced iron ratio.

While it can be seen that the reduced iron ratios estimated using the basic atomic formula method do not yield unique and entirely accurate values they are consistent with the value of the actual ratio. Results for the same analyses obtained using the four cation bases are given in Table 3.4 and illustrated in Fig 3.7. It can be seen that none of the cation bases are consistent in indicating the 'correct' (actual) reduced iron ratio. In particular it is worthy of note that the $\sum FM = 13$ cation base (Fig. 3.7d) tended to give values for the reduced iron ratio which in almost every instance were too high (ferrous rich). It is suggested therefore that the basic atomic formula method of estimating the iron oxidation ratio described

Table 3.4. Comparison of the actual and calculated reduced iron ratios for a number of amphibole analyses taken from the amphibole data file.

a base erence ber*	Actual reduced iron ratio	Calculated reduced iron ratio (basic atomic formula)	Calculated reduced iron ratio (cation bases.) $\sum$Na=16	$\sum$Na=15	$\sum$Ca=15	$\sum$FM=13
09	0.52	0.50-0.72	1.0	0.55	1.0	0.55
91	0.79	0.88-1.0	1.0	0.75	1.0	1.0
92	0.82	0.78-1.0	1.0	0.71	1.0	0.81
93	0.83	0.70-1.0	1.0	0.23	0.94	0.70
94	0.66	0.60-1.0	1.0	0.37	1.0	0.71
04	0.78	0.80-1.0	1.0	0.30	1.0	1.0
13	0.70	0.57-0.95	1.0	0.20	0.98	0.85
30	0.71	0.57-0.92	1.0	0.0	0.84	0.80
47	0.56	0.92-1.0	0.98	0.0	1.0	0.94
35	0.68	0.55-0.65	0.86	0.0	1.0	0.93
37	0.79	0.77-1.0	1.0	0.34	1.0	0.93
39	0.72	0.72-0.97	1.0	0.0	0.97	0.86
39	0.67	0.57-0.87	0.87	0.0	1.0	0.70
14	0.76	0.92-1.0	1.0	0.12	1.0	0.96
32	0.80	0.62-0.97	1.0	0.35	0.95	0.83
58	0.79	0.72-1.0	1.0	0.25	1.0	1.0
39	0.86	0.85-1.0	1.0	0.75	1.0	1.0
38	0.81	0.67-0.97	1.0	0.27	0.98	0.83

$\sum$Na=16, Cation base of 16 cations, A site full.

$\sum$Na=15, Cation base of 15 cations, A site vacant.

$\sum$Ca=15, All cations except Na^+ and presumably K^+ normalised to 15.

$\sum$FM=13, All cations normally present in thy Y and Z groups normalised to 13.

*Details of the source of the analyses can be obtained from Appendix 8.

Fig. 3.6. Comparison of the reduced iron ratios calculated from the basic atomic formula with the actual reduced iron ratios of a number of amphibole analyses taken from the amphibole data file.

Calciferous and alkali amphiboles are indicated by a solid line, and amphiboles outside amphibole compositional space by a dashed line.

The diagonal line corresponds to equal actual and estimated reduced iron ratios.

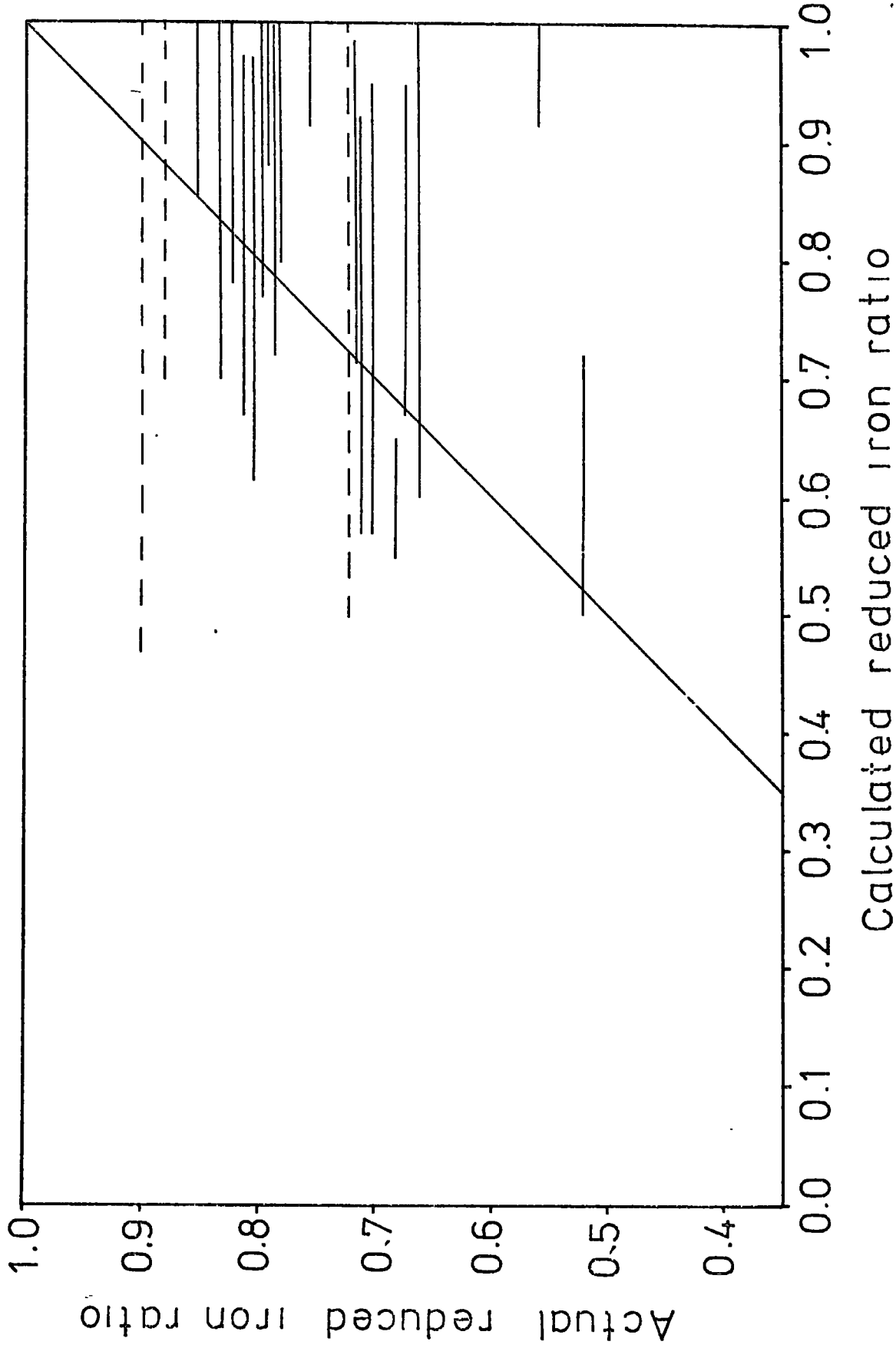
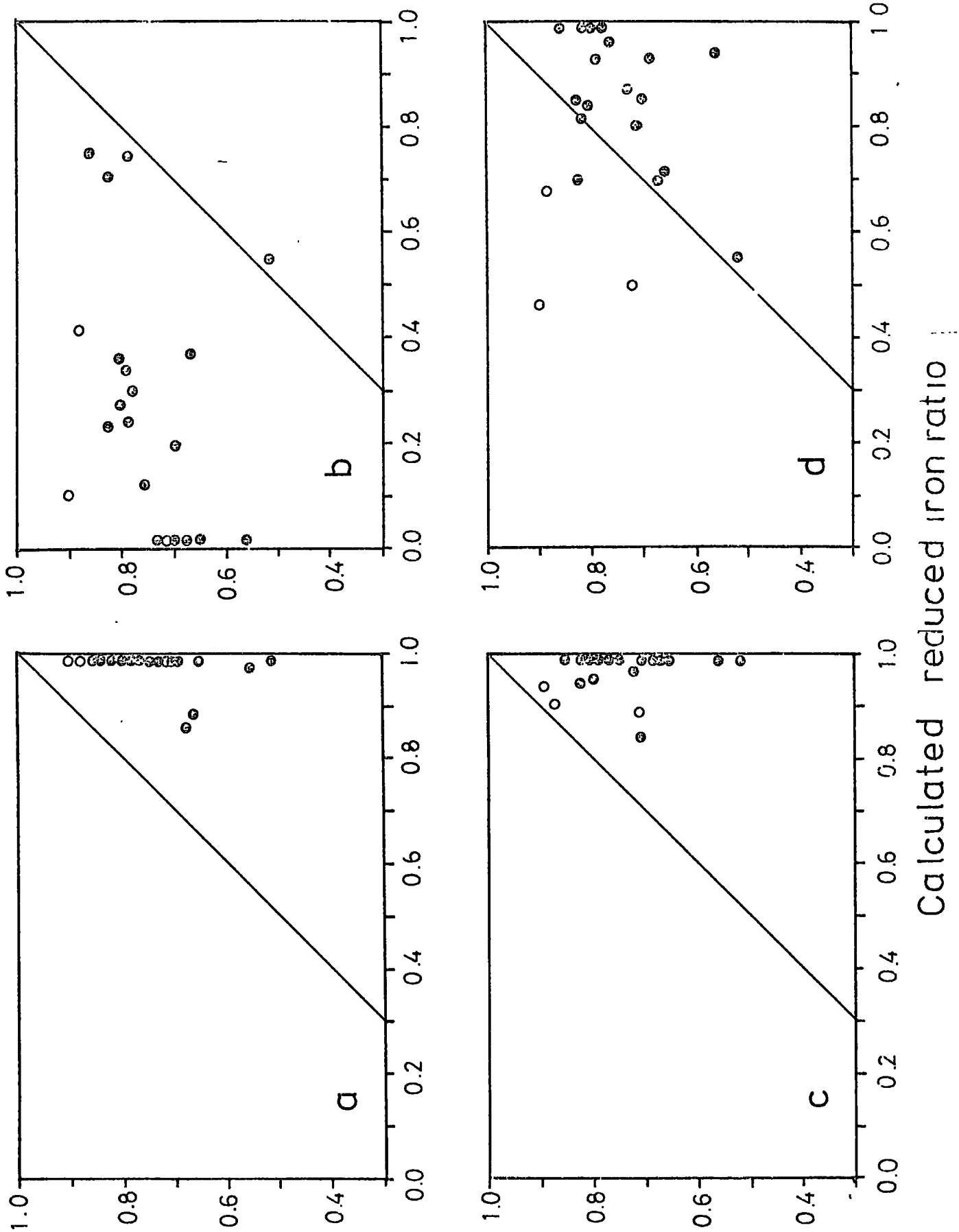

Actual reduced iron ratio
1.0
0.9
0.8
0.7
0.6
0.5
0.4
Calculated reduced iron ratio
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Fig. 3.7. Comparison of the actual and estimated reduced iron ratios calculated from four cation bases.

The nomenclature of the cation bases is the same as Fig. 3.5.

Calciferous and alkali amphiboles are indicated by closed circles, and amphiboles outside amphibole compositional space by open circles.

The diagonal line corresponds to equal actual and estimated reduced iron ratios.


Actual reduced iron ratio
Calculated reduced iron ratio
a
b
c
d
0.0
0.2
0.4
0.6
0.8
1.0

above is as good as, and probably superior, to alternative cation bases.

As mentioned in Section 3.1 the method described here is applicable only to amphiboles in which the hydroxyl group is fully occupied by OH^-, F^-, or Cl^- and which belong to the calciferous or alkali amphiboles. Attempts to extend the method to amphiboles with even minor amounts of Y group cations in the X group at the 'correct' oxidation state (or reduced iron ratio) results in extended ranges of reduced iron ratios consistent with $(Na^A + Al^Y) = (Na^X + Al^Z)$. To illustrate this, three such amphiboles, analyses 289, 1480, 1627 (for details see Appendix 8) with respectively 0.21, 0.09 and 0.21 Y group cations in the X group have been plotted on Fig. 3.6 (dashed lines). In each instance the range of estimated reduced iron ratios is large and extends to values considerably lower than the original.

This behaviour may be attributed to the transfer of cations from the Y to the X group. In Section 3.1.3 it was shown that for amphiboles in amphibole compositional space this event resulted in almost all compositions having $(Na^A + Al^Y)$ equal to $(Na^X + Al^Z)$ for all higher reduced iron ratios. For compositions outside amphibole compositional space this situation will occur at reduced iron ratios lower than the actual value and explains the extended range of possible reduced iron ratios. Ratios calculated for the same analyses using the cation bases (open circles Fig. 3.7) indicate that cation bases are also unsuccessful in coping with such situations.

Examination of Fig. 3.4 indicates that using the basic atomic formula method the range of possible reduced iron ratios extends in a number of instances to 1.0 even though the actual value was lower. This introduces an interesting corollary of using the basic atomic formula method to estimate oxidation states. The mere balance of the basic atomic formula of an electron microprobe analysis of an

amphibole with all iron reported as FeO (reduced iron ratio = 1.0) does not necessarily imply that there is only (trivial amount) Fe_2O_3 present.

4. A COMPUTER DATA FILE FOR THE AMPHIBOLES.

As part of the study of the chemistry of the amphiboles it was decided to collect as many published and unpublished analyses of amphiboles as was feasible. A total of 2650 analyses was obtained and it soon became obvious that a computer data file would be required to cope with such a large amount of data. The collection, transcription and punching of any large body of information is a costly and time consuming operation. Often in the past the resultant data file has been of interest only to a limited number of other users. It was envisaged at the outset that a data file of information about amphiboles would be of interest to mineralogists, igneous and metamorphic petrologists provided the information concerning individual amphiboles was extensive. To accomplish this as much information as possible about each specimen has been included in the data file. To be of maximum value as a secondary source of information the data in the data file should be in a form as close to the original as possible. This necessitates the use of a versatile data base.

In Section 4.1. the merits of various types of data bases which can be implemented in FORTRAN or PL/1 are described. Experience with a data base written in PL/1 by the author is discussed briefly. Thanks to the generosity of Dr. M.G. Notley of the IBM United Kingdom Scientific Centre it has been possible to implement the amphibole data file under a prototype general data base strategy. The generality of the data base is demonstrated for geological data with examples from stratigraphy and mineralogy. In Sections 4.2 to 4.4 the implementation of the amphibole data file is described.

4.1. Choice of a data base strategy.

The following can be recognised as basic requirements of a successful data base.

1) The data base should be capable of handling any data in a manner

as close to the external form and organisation as possible.

2) The form in which the data is stored should not inhibit the setting of meaningful queries.

3) Once created the data base should be simple to update delete, etc. and be efficient in time and storage, or both.

Requirement (1) deserves more attention. Two aspects are important. Firstly, to be of the greatest value data included in the data base should be in a form as close to its original as possible (Hubaux 1969, p. 49). The use of often arbitary codes, fixed vocabularies, etc. should be avoided as this imprints the prejudices and opinions of the coder onto the data and requires the use of bulky books of codes. For examples of these see Harrison & Sabine (1970) and Chayes (1972). The maintenence of the data in a form close to the original is taken here as a major objective. Secondly, to comply successfully with requirements (1) and (2) the data base must be designed around an appropriate 'model of information'. By 'model of information' is meant an attempt to recognise and preserve the inherent structure of the external form of the data within the data base itself.

In the simplest case mineralogical data consists of a number of 'objects' with various 'properties' (characters or attributes) which can have 'responses'. The responses can be in either alphanumeric, integer or floating point mode. Take for example the mineral tremolite as an object. It may possess, among others, the following properties:-

(1) SiO_2, MgO, CaO, ---------- etc.

Eu, Cu, Zr, ---------- etc.

r.i. α , r.i. β , r.i. γ , 2V.

Pleochroic scheme X, Y, Z.

---

etc.

More complicated situations arise in which there is more than one possible response for a property. That is to say the responses are not mutually exclusive. The X axis of the pleochroic scheme may simultaneously take responses of the type 'yellow' and a quantitative indication of the colour.

4.1.1. Vector organisation.

The simplest model of information of properties P_1 to P_n and responses R_1 to R_n is in the form of a vector (2).

(2)

	P1	P2	—	—	—	—	—	Pn
Object	R1	R2	—	—	—	—	—	Rn

Vectors are very convenient for computer processing. This is especially the case if the mode of all the responses is always the same. The external vector organisation can be transferred directly to an internal vector organisation. Sequences of vectors each with the same number of properties in the same order and all of the same data mode may be incorporated into two dimensional arrays. Array handling facilities are efficient in programming languages.

In general all the responses are not of the same data mode, in example (1), the pleochroic scheme, X, Y, Z, are character strings, the refractive indices and the major elements are non-integers and the trace elements either integers or non-integers. Data of this type can still be considered as vectors externally and may be processed in a sequential manner but the programming involved is somewhat more complicated than when responses are all in the same mode.

Many forms of geological data have been made to comply with vector organisation. Possibly the best known examples, both in igneous petrology, are RKFNSYS, (Chayes 1972) and CLAIR, (LeMaitre

1973). Vector organisation has been used extensively because of its simplicity from a computational viewpoint (Loudon 1970).

The disadvantages in the use of vectors stem from three sources, (i) data dependence, (ii) data redundancy and (iii) the vector may be an inappropriate model of the external organisation of the data. Considering the first two points together. At the outset of any data collection process all the possible properties for which information is to be stored must be recognised. This is because the processing programs are normally dependent upon the number, mode and order of the responses. The insertion of an additional response involves alterations in the processing programs. The outcome of having to recognise all the possible properties of a group of objects in advance is a large number of properties only a few of which ever take responses for any individual object, and hence a high level of data redundancy. Taking as an example a vector organisation to represent the optical properties for silicate minerals, to include every possibility each vector must contain the properties, n, o, e, α, β, and γ, refractive indices. A high level of data redundancy is involved. Worse still the no responses are of two types, some represent 'not determined' e.g. α, β if γ determined, others 'not appropriate' e.g. n, o, e, if β determined.

4.1.2. Tree organisation.

Closer examination of mineralogical data indicates that a hierarchical structure is present. Hierarchical structures are normally referred to as 'trees' (Loudon 1970). The properties of the silicate mineral in (1) may be shown in the form of a tree, see Fig. 4.1.

In a tree the following notation is used:

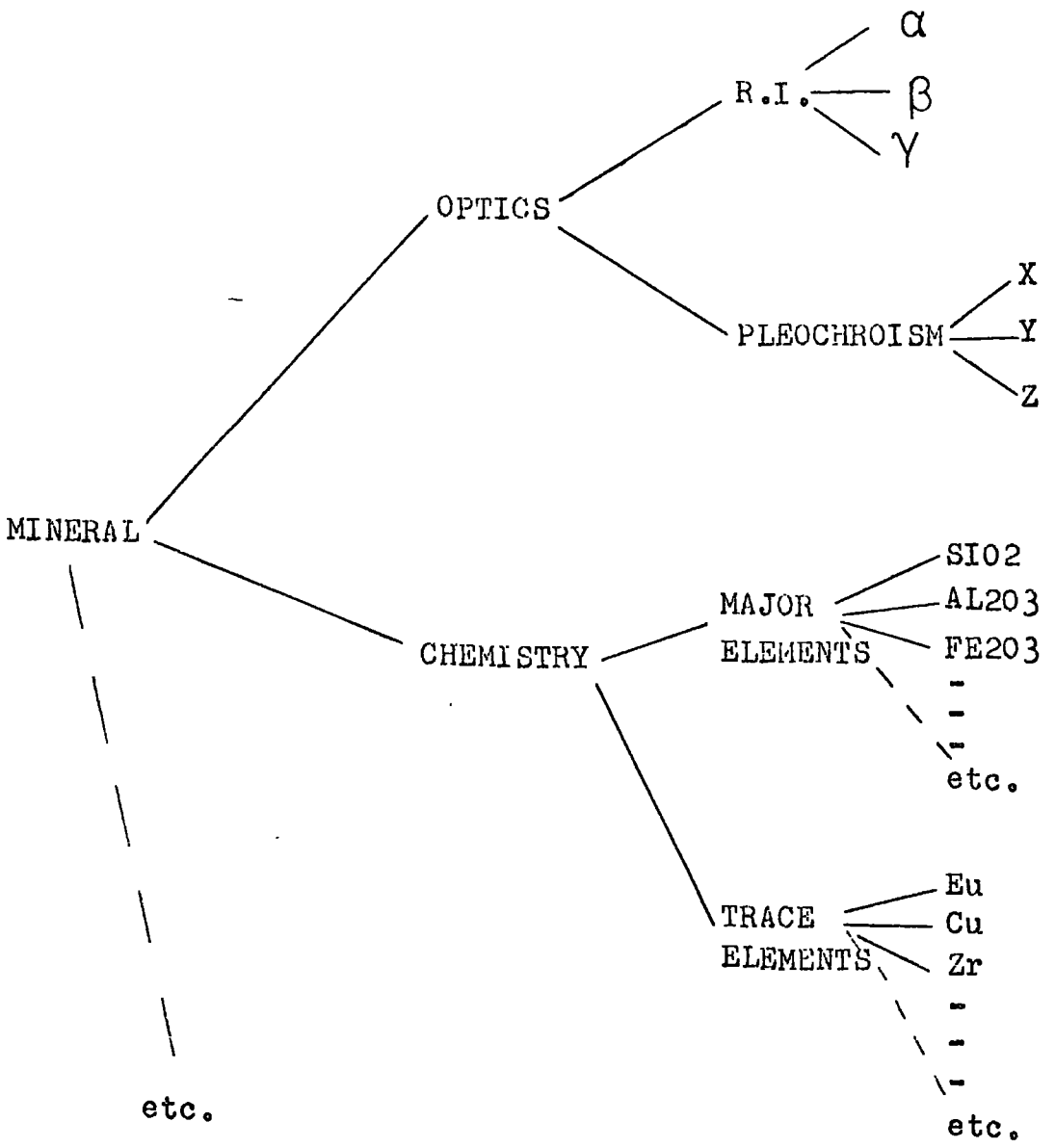
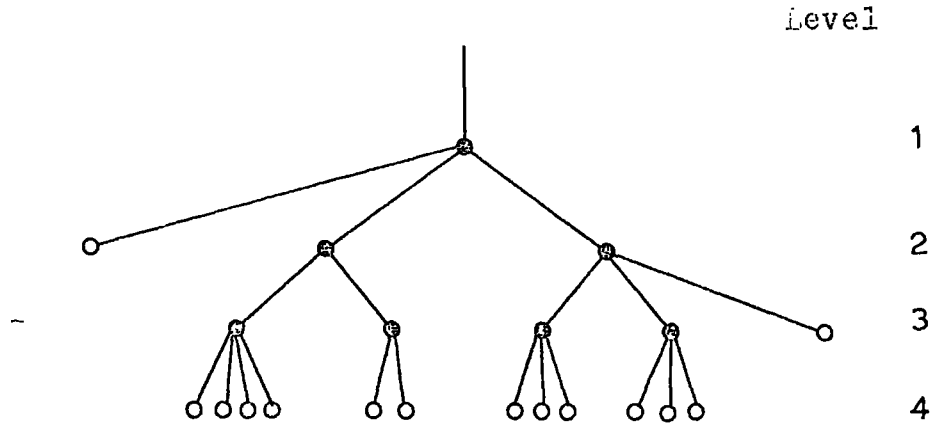


Fig. 4.1. A hierarchical, or tree, organisation of some properties of a silicate mineral.

(3)



⊛ node.

o elementary level.

Responses to properties can only be entered in the elementary levels. Nodes indicate the inter-relationship between elementary levels and other nodes, they themselves can not take responses.

If the external form of the data is in a hierarchical form many of the queries are themselves hierarchical in nature. There is an advantage therefore if the internal organisation is also hierarchical. Suppose for the sake of an example a query asking for all the major element chemistry for a mineral is set. If the data is organised in a non-hierarchical manner it is necessary to define explicitly in the query which properties are included in 'major elements'.

High level programming languages, for example PL/1, offer hierarchical facilities. The form of the tree, the mode of the elementary levels and the nomenclature of the elementary levels and nodes is defined explicitly. Unlike arrays there is no limitation on the use of mixed modes at elementary levels. In fact a PL/1 structure of only two levels may be considered as a vector with mixed modes. Data manipulation can be made in terms of the whole structure, part of the structure, or elementary levels. The main advantage in a PL/1 structure lies in the ability to cope easily with data of mixed mode. However like arrays PL/1 structures are explicitly

defined and are of fixed shape and length which leads in turn to data dependence and large scale data redundancy. In addition queries can only be set of the elementary levels individually and not of nodes so that a hierarchical query is impossible.

To avoid the difficulties of data redundancy and data dependence a data base was written in which storage space is not allocated unless a response is actually present and the data structure (provided it is a tree) is independent of the loading and query programs. In the case of the amphibole data file a large and complex tree was used as the data structure (Table 4.1).

A data structure in the form of a tree is defined externally to the loading and query programs which then become independent of the data structure in vogue at any time. This is accomplished by describing the nodes and elementary levels in an n - level tree in terms of a unique combination of n-1 integers, Fig. 4.2. These n-1 integers define the hierarchical inter-relationships of the elementary levels and nodes. For each node or elementary level the n-1 level numbers, property name and the data mode are read into the loading program (see Appendix 5 for details). Thus for example the entry for the elementary level COUNTRY (Fig 4.2) which is alphanumeric (mode = 1) is 1,1, COUNTRY,1. Alternative names for nodes and elementary levels are allowed but duplicate names are not.

Each item of data (response) consists of three parts, (i) the reference number of the object, so that data concerning the same object can be recognised, (ii) the name of the elementary level to which the data are to be directed, (iii) the response itself. Thus the country of origin of object number 47 is input as:- 47, COUNTRY, ENGLAND. In the loading program the elementary name is matched with the names in the data structure and replaced by n-1 level numbers.

Table 4.1. Proposed hierarchical structure for the amphibole data file.

LEVEL 1	LEVEL 2	LEVEL 3
AMPHIBOLE REFERENCE		AUTHOR, AUTHOR_INITIALS, ANALYST, ANALYST_INITIALS, DATE, JOURNAL.
GEOGRAPHY		COUNTRY, COUNTY, LOCALITY,
HOST_ROCK		
MINERAL_NAME		
OPTICS		ALPHA, ALPHA_ERROR, BETA, BETA_ERROR, GAMMA, GAMMA_ERROR, DELTA, DELTA_ERROR, 2V, DISPERSION, ORIENTATION, O.A.P., EXTINCTION_ANGLE.
ELECTRONICS		FORMULA, X, Y, Z,
BODY_CYCLE		
STRUCTURE		A, A_ERROR, B, B_ERROR, C, C_ERROR, BETA, BETA_ERROR, VOLUME, SPACE_GROUP,
PHYSICAL_PROPS.		DENSITY, HARDNESS,
MAJOR ELEMENTS		AL2O3, AS2O3, B2O3, BAO, BEO, CAO, CDO, CL, CRO, CR2O3, CUO, F, FEO, FE2O3, K2O, LI2O, MNO, NA2O, NIO, P2O5, PBO, S, TIO2, V2O3, ZNO, ZRO2, TOTAL,
TRACE_ELEMENTS		AS, BA, BI, BE, CD, CE, CL, DY, ER, EU, FR, GA, GD, HF, LA, LI, LU, NB, ND, MO, PB, SB, SC, SM, TB, TM, Y, YB, YT,
TECHNIQUE		ANALYTICAL_METHOD, ADDITIONAL_TECHNIQUES,
COEXISTENCE		FIRST_AMPHIBOLE, SECOND_AMPHIBOLE, THIRD_AMPHIBOLE,
EXTRA_DATA		
RECOMBINATION,		

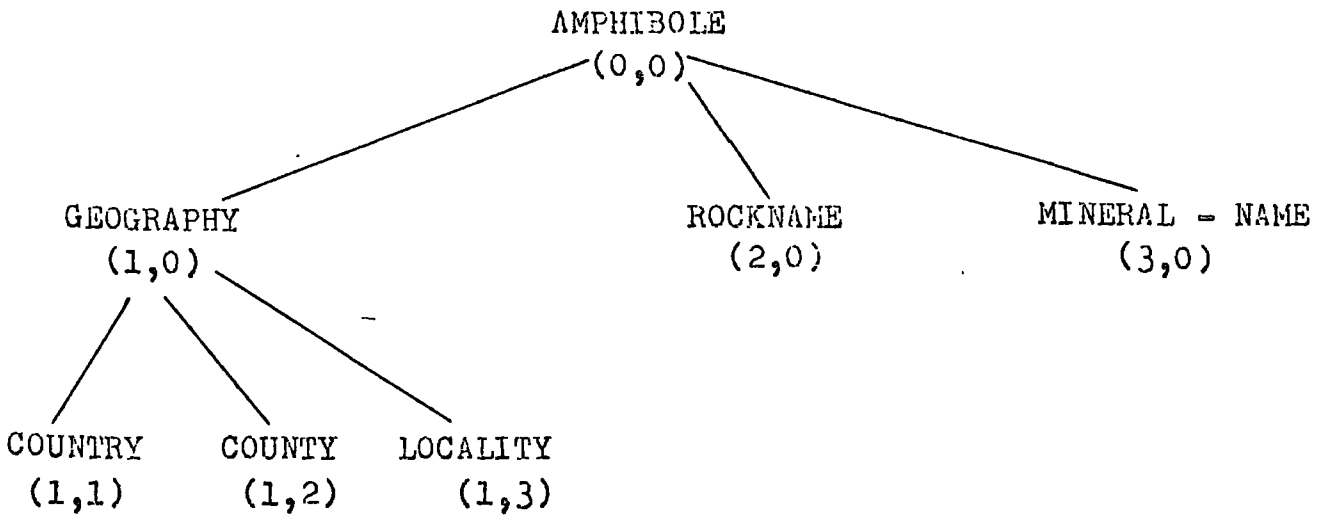


Fig. 4.2. An example of a three level structure showing the derivation of level numbers for the nodes and elementary levels.

To save storage space the n-1 level numbers are combined uniquely into a single composite integer value and the response stored sequentially in four parts, the object number, the compound level number, the data mode, and the response. By using integers the amount of storage space required is reduced. In theory the mode need not be stored.- In this way 'no responses' are not stored and a hierarchical structure is retained in terms of the level number.

Queries of the data are undertaken by a query program (Appendix 5) in which the query in the form of a modified 'IF statement' and the names of the fields for which data is to be output are read in as data. The program acts as a simplified compiler and interprets and sets the query. In this way the program is independent of the data structure and the query.

As mentioned above the major advantage of such a data base lies in its ability to cope with data redundancy and data dependence. Provided the proportion of 'no responses' inherent in the data are large the extra storage required for the integer object number, compound level number and data mode are likely to be less than the storage of 'no responses'. Examination of Table 4.1, shows that a large and complex tree is required for the amphibole data file and experience has shown that, on average, responses occur in only 25 per cent of the elementary levels for each amphibole. It would appear therefore that the data base is well suited to the amphibole data file. The data independence of the loading and query programs allows additional responses to be added without altering the programs and provided the level numbers of existing nodes and elementary levels are not affected without having to reload the data. Although not implemented, simple presence / absence queries of a hierarchical nature could be set.

The major disadvantage of the data base is that it is not particularily efficient in time. This may be attributed to the use of a high level programming language and the necessity of searching through all the data in a sequential manner to obtain responses to queries. Loading of large amounts of data is tedious in that the name of the elementary level must be specified for each response. The work involved can be reduced by either (i) specifying an equivalent but shorter name for the elementary level or (ii) modifying the loading program so that if large numbers of responses for the same properties in different objects are to be input the elementary level name need not be repeated. However this latter modification has not been undertaken because soon after the data base was written a more versatile general data base strategy became available for use by the author (Section 4.1.3).

4.1.3. Relational organisation.

While a hierarchical view of the external form of data is satisfactory for mineralogy it is not satisfactory, or applicable, to every branch of geology. In many forms of geological data it is not true to simply state, as previously, that data consists of a series of 'responses' to 'properties'. Often complex spatial or temporal relationships exist. Consider for example statements of the type:-

(5)

B overlies A and both are intruded by C.

The order of crystallisation was X, Y and then Z.

Information of this type Dixon (1970) termed 'natural geological structure', and suggested that it could be interpreted in terms of a relationship between objects A and B of the sort :

OVERLIES (B, A)

A completely general data base strategy capable of handling just such relationships using a relational model of data

was first suggested by Codd (1970). While a relational model of data is able to describe 'natural geological structure' it will be shown in the following paragraphs that the model is applicable to geological and mineralogical data in general. A working prototype data base incorporating a relational model of data became available for use by the author in 1972. The data base has been described by Notley (1972) and is at present implemented at the IBM United Kingdom Scientific Centre, Peterloo, Co. Durham. The amphibole data file has been implemented using this relational model, see Roper, Osmen & Knight (1973). A brief description of the relational model is given below. For a more detailed account see Codd (1970) and Notley (1972). While a relational model of data is new to the geological sciences a great deal of present day research on computer data bases is following a similar approach (e.g. Chamberlain & Boyce 1974; Steuert & Goldman 1974).

Within any body of data objects may be recognised. (Note that objects may themselves consist of numerous responses to properties In a later section properties and responses will be shown to take the same role as objects in the present context). Using the examples in (5) A , B , C, and X , Y , Z, are objects. A relationship is an association of more than one object. The relationship 'overlies' holds between objects A and B. The objects making up a relationship are called a tuple and the number of objects in a tuple its degree, two in this case. A relation, as opposed to a relationship, is a collection of every valid instance of a specific relationship. The relationship 'intrudes' holds between C and A, and between C and B. Provided the objects in each tuple are in the same order a relation may be envisaged as a data table (6). The rows are

(6) INTRUDES (INTRUSION, COUNTRY-ROCK)

C	A
C	B

tuples and the columns are termed domains. The number of tuples is called the cardinality of the relation. Normally the domains are given unique names as (6). Provided there is no duplication of tuples and their ordering is immaterial the table may be considered a relation in its mathematical sense and a powerful series of set operations become available for use. For a simple discussion of set operations see Appendix 6 and Notley (1972). A more detailed discussion of set operations may be found in Codd (1970).

As an illustration of the use of the relational model of data to describe complex inter-relationships, the relations required to describe the information present in the stratigraphic column, Fig. 4.3, are given in Table 4.2. By applying set operations it is possible to set complex queries of the data in relational form. As an example consider the query, 'what is the age of rocks intruded by both X and Y ?'. One of the possible alternative ways of setting the query in terms of set operations is :-

Select from INTRUSION all rocks intruded by X.

SELECT (IGNEOUS-ROCK = X) yields

A (IGNEOUS-ROCK, COUNTRY-ROCK)

X	A
X	B

Select from INTRUSION all rocks intruded by Y.

SELECT (IGNEOUS-ROCK = Y) yields

B (IGNEOUS-ROCK, COUNTRY-ROCK)

Y	B
Y	C
Y	D

Take a projection of relations A and B on domain

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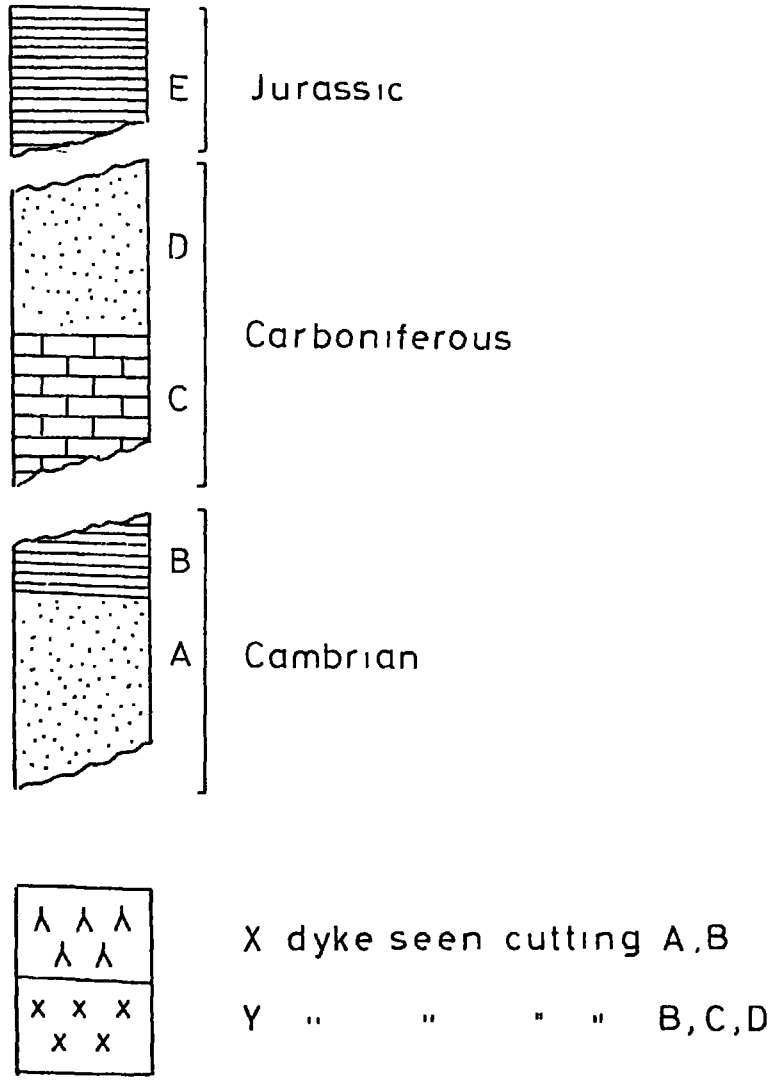


Fig. 4.3. A simplified stratigraphical column.

Table 4.2. Relation necessary to describe completely the data in the stratigraphic column illustrated in Fig. 4.3.

OVERLIES (LOWER-STRATUM, UPPER-STRATUM)

A	B
C	D

UNCONFORMITY (LOWER-STRATUM, UPPER-STRATUM)

B	C
D	E

INTRUSION (IGNEOUS-ROCK, COUNTRY-ROCK)

X	A
X	B
Y	B
Y	C
Y	D

EQUALS (NAME, PROPERTY, VALUE)

A	AGE	L.CAMB.
A	ROCKTYPE	SANDSTONE
B	AGE	U.CAMB.
B	ROCKTYPE	SHALE
C	AGE	L.CARB.
C	ROCKTYPE	LIMESTONE
-	-	-
-	-	-
-	-	-
-	-	-
etc.	etc.	etc.

COUNTRY-ROCK. (The command for a projection is termed REORDER, see Notley 1974).

REORDER (COUNTRY-ROCK) reln. A gives C (COUNTRY-ROCK)

A

B

reln. B gives D (COUNTRY-ROCK)

B

C

D

Find the intersection (i.e. common tuples of C and D)

INTERSECT yields E (COUNTRY-ROCK)

B

The age of B can be found by a selection of relation EQUALS

SELECT (PROPERTY = AGE & NAME = B)

yields the result

B (U. CAMBRIAN).

So far the relational model has been described for a stratigraphical example. The problem now arises as to whether the model is applicable to mineralogical data. Consider for example the major elements in a silicate chemical analysis. It is possible to include these in two types of relations.

(9a) EQUALS (PROPERTY-NAME, RESPONSE)

SI02	44.99
AL203	11.21
FE203	3.33
- - -	- -
etc.	etc.

(9b) (SI02, AL203, FE203, - - , - - , etc.)

44.99 11.21 3.33 - - , - - , etc.

- - - -

etc.

In the first of these there is a semantic relationship between the domains, in the second there is only a dummy relationship. Both are relations in the mathematical sense (data table with unique rows, in which row ordering is immaterial). For convenience both relations may be termed MAJOR-ELEMENTS or some other meaningful name.

It has been argued that mineralogical data displays a hieracrchial structure. As can be seen from (9b) a relation may be defined in such a manner as to display at least limited hierarchical structure. Data manipulation can be made in terms of domains or the relation as a whole. However, at least in theory, within a relation domains can themselves be relations thus representing a hieracrchical structure, see (10).

(10) OPTICS (SPEC.# , PLEOCHROISM, COLOUR, R.I.)
PLEOCHROISM (SPEC.# , X, Y, Z)
COLOUR (SPEC.# , COLOUR)
R.I. (SPEC.# , α , β , γ)

In general much simpler data representation is possible if relations without hierarchical domains are used. Codd (1970, 1971) has suggested methods for deriving relations with simple domains from a hierarchical collection of relations. In the present context it has been found that sufficient hierarchical structuring can be achieved by a judicious choice of the definition of relations, see Section 4.3.

A data base incorporating a relational model of data has been implemented at the IBM United Kingdom Scientific Centre. Data is stored in relations. The relation name, domain names and mode are defined by the user outside of the data base. Queries of the relational data base are written in a simple query language incorporating set operations (Appendix 6). In addition commands to load, store and list relations as well as commands to start or terminate a query are required. These are described by Notley (1972). Apart

from the simple nature of queries the relational model allows complete data independence (Roper, Osman & Knight 1973) and by a judicious choice in the definition of relations data redundancy can be limited.

4.2. Scope of the data included in the amphibole data file.

To be of value in the envisaged use of the data file (Chapter 1), information relating to any amphibole must include at least a 'major element chemical analysis'. This is defined as one with silica plus at least three other major elements. Apart from this no further distinction has been made on the usefulness or accuracy of the included data. This was part of a deliberate attempt to retain the amphibole data file as a secondary source of information free from the prejudices of the coder.

The scope of the data included in the data file is described below.

a) Literature Reference.

This includes the author's surname and initials plus those of the analyst if known. If there is more than one author each is included separately as a joint author of the paper. Date of publication, journal name, volume and page numbers are included where appropriate. In those instances in which a particular analysis was designated by an identifier in the original source this is also included.

b) Mineral Name.

The name given to the mineral by the author.

c) Geographical Information.

Includes the country, state, province or county and the exact locality of the specimen.

d) Petrological Information.

Because of the difficulties and time involved in

interpreting the available petrological information (see Chapter 8) only the authors name for the host rock was included.

e) Optical Properties.

In transmitted light, the α, β, γ, refractive indices and their errors of determination, magnitude and sign of the optic axial angle, and orientation of the indicatrix, pleochroic scheme and absorption formula were all recorded.

f) Chemical Information.

Major elements with values in weight per cent and trace elements in ppm were included.

g) Techniques.

Information regarding the analytical technique employed was recorded along with the application of techniques, such as infrared and Mössbauer spectroscopy which otherwise yield information not included in the data file.

h) Physical Properties.

The hardness, density and specific gravity were included.

i) Structural Properties.

Space group symmetry, unit cell parameters A, B, C, β, volume and their errors of measurement.

j) Cross-referencing Information.

Three different forms of cross-referencing between individual amphiboles specimens were recognised, each implying that some further information in the data file is relevent to the specimen under consideration. The three recognised forms are, (i) the addition of extra data to an item already in the data base, (ii) the re-determination of properties of a specimen already in the data file, (iii) reference to amphiboles which are known to coexist with the specimen under consideration.

4.3. Definition of a relational framework for the amphibole data file.

In setting up a relational framework to include the considerable scope of data in the amphibole data file, relations were defined so as to keep closely related data together. Thus for example the relation GEOGRAPHY includes the scope of the geographical information. (The meaning of the REF.NO. is considered below. Because each

GEOGRAPHY (REF.NO., COUNTRY, COUNTY, LOCALITY)

of the domains is to be expected to contain approximately equal numbers of responses, data redundancy is limited. However, in those instances in which responses are not equaly common across all the domains, closely related data has been distributed between more than one relation to limit data redundancy. An example of this is the specimen number given to the amphibole analysis by the original author. The number of responses was considerably less than the remaining reference information and so two separate relations REFERENCE and ANALYSIS were set up.

REFERENCE (REF.NO. , AUTHOR, AUTHORINITIALS, ANALYST, ANAIYSTINITIALS, DATE, REFERENCE, VOLUME)

ANALYSIS (REF.NO. , REF. CODE)

Lastly, where data redundancy is high and there are a very large number of possible properties, as in major and trace element chemistry, relations of the general type

name (ref.no., property, response)

have been used. The complete collection of relations as originally defined is given in Table 4.3.

Using MINDATA5 (Appendix 4) atomic formulae and basic atomic formulae were calculated for all the analyses and the results stored in two additional relations organised as (9b). The organisation of these relations is highly wasteful of storage but it was felt that this was justified so that this data could easily be processed as vectors by a -

RELATION NAME	DOMAIN NAME
REFERENCE	REF.NO.
	AUTHOR
	AUTHORINITIALS
	ANALYST
	ANALYSTINITIALS
	DATE
	REFERENCE
	VOLUME
ANALYSIS	REF.NO.
	REF.CODE.
MINERALNAME	REF.NO.
	NAME
GEOGRAPHY	REF.NO.
	COUNTRY
	COUNTY
	LOCALITY
OCCURRENCE	REF.NO.
	ROCKNAME
OPTICS	REF.NO.
	ALPHA
	ALPHAERROR
	BETA
	BETAERROR
	GAMMA
	GAMMAERROR
	2V
	DISPERSION
	ORIENTATION
	O.A.P.
	DELTA.
	DELTAERROR
	EXT.L.

Table 4.3. Relation and domain names used in the amphibole data file.

RELATION NAME	DOMAIN NAME
OCCUR	REF.NO. OCCUR
PLEOCHROISM	REF.NO. FORMULA X Y Z
CHEMISTRY	REF.NO. OXIDE VALUE
TRACE	REF.NO. ELEMENT VALUE
TECHNIQUE	REF.NO. EXAMINATION ANALYTICAL_METHOD
PHYSICAL	REF.NO. PROPERTY VALUE
STRUCTURE	REF.NO. CELLPARAMETER VALUE ERROR
SYMMETRY	REF.NO. SYMMETRY
COEXISTENCE	REF.NO. OTHER_REF.NO.
EXTRA	REF.NO. OTHER_REF.NO.
REDETERMINATION	REF.NO. OTHER_REF.NO.

number of statistical and plotting programs, (Chapters 6, 7 and 8). With the present implementation of the relational data base the mode for each domain, once defined, must remain the same. A complete list of the data characteristics for each of the relations is given in Appendix 7.

As part of the definition of a relation each tuple must be unique. Examination of the relations in Table 4.3 suggests that this in general will not be the case. For simplicity each amphibole specimen has been identified by a unique integer (REF.NO.) starting at unity and increasing in the order of acquisition. The reference number has been included as a domain in all the relations. It renders tuples unique and acts as a method of cross-referencing between relations.

No claim is made that these relations are the optimum ones to describe the data succinctly and yield fast response times to queries. However, one of the major advantages of the relational model as implemented is the ability of the computer to re-arrange the data in relations to bring about such optimisation. This aspect of the relational model of data has been the subject of study by Osman (1974).

4.4. Data capture, transcription and validification.

The methodology behind data capture and a complete list of the sources of data in the amphibole data file are given in Appendix 8. A detailed description of the method used in transcribing data is given in Appendix 9. Throughout, the use of arbitary codes has been avoided and the data is in a form as similar to the original as possible.

In all, data relevant to 2650 different amphiboles has been included in the data file at present. This collection is by no means exhaustive, with the emphasis on English language sources, see

Appendix 8. However, it is considered that the collection is probably representative of the chemical variation exhibited by the amphibole group.

Care was taken during the transcription process to encode the source material accurately. All punched cards were listed and the listing compared visually with the coding sheets. Violations of data modes or lengths were detected on adding data to the data base. Offline programs, written in PL/1, interfacing directly with the data base, were written to locate internal inconsistencies in the data. The encoded analysis TOTAL was compared with the sum of the major elements of the appropriate analysis in relation CHEMISTRY. A discrepancy in excess of 0.01 per cent, after allowing for oxygen equivalences of F, Cl, was taken as an error. By far the majority of 'errors' located in this manner turned out to be due to inaccurate analysis totals in the literature rather than transcription errors.

Similarly in relation OPTICS, a program was written to locate internal inconsistencies in the optical data which may have been attributed to transcription errors. Four checks were carried out :-

1) $\alpha \neq \beta \neq \gamma$

2) $\alpha < \beta < \gamma$

3) The sign of the optic axial angle calculated from the refractive indices by equations +ve $\frac{1}{\alpha^2} - \frac{1}{\beta^2} < \frac{1}{\beta^2} - \frac{1}{\gamma^2}$

-ve $\frac{1}{\alpha^2} - \frac{1}{\beta^2} > \frac{1}{\beta^2} - \frac{1}{\gamma^2}$

was compared with the observed sign.

4) The observed value for the 2V was compared with the value calculated from the refractive indices using equations.

$$\tan^2 V_\alpha \frac{\alpha^2(\gamma^2-\beta^2)}{\gamma^2(\beta^2-\alpha^2)} , \qquad \tan^2 V_\gamma \frac{\gamma^2(\beta^2-\alpha^2)}{\alpha^2(\gamma^2-\beta^2)} .$$

In general it is to be expected that the observed and calculated value for the optic axial angle will be similar but not necessarily identical. This is because the refractive indices and 2V are determined independantly and are each prone to errors of measurement. The method of comparison used involved calculating the range of 2V's consistent with the observed refractive indices and their errors of measurement calculated from simple theory for the error of a compound quantity (Topping 1962) and comparing this range with the observed 2V.

Transposing equations for the 2V to the form

$$2V_\alpha = 2.\arctan\sqrt{\frac{\alpha^2(\gamma^2-\beta^2)}{\gamma^2(\beta^2-\alpha^2)}} , \qquad 2V_\gamma = 2.\arctan\sqrt{\frac{\gamma^2(\beta^2-\alpha^2)}{\alpha^2(\gamma^2-\beta^2)}}$$

and assuming that the errors $e\alpha$, $e\beta$ and $e\gamma$ in the determination of the refractive indices are independant and small compared with their respective refractive indices then the fractional errors are given by

$$f\alpha = \frac{e\alpha}{\alpha} , \quad f\beta = \frac{e\beta}{\beta} , \quad f\gamma = \frac{e\gamma}{\gamma} .$$

The approximate maximum total fractional error F is given by

$$F = f\alpha + \frac{\gamma^2 f\gamma \quad \beta^2 f\beta}{\gamma^2-\beta^2} + f\gamma + \frac{\beta^2 f\beta \quad \alpha^2 f\alpha}{\beta^2-\alpha^2}$$

let $$X = \sqrt{\frac{\alpha^2(\gamma^2 - \beta^2)}{\gamma^2(\beta^2 - \alpha^2)}}$$

and $$Y = \sqrt{\frac{\gamma^2(\beta^2 - \alpha^2)}{\alpha^2(\gamma^2 - \beta^2)}}$$

then the approximate maximum range calculated for 2V is given by

(4a) $$2V_\alpha = 2 \cdot \arctan (X \pm F)$$

(4b) $$2V_\gamma = 2 \cdot \arctan (Y \pm F)$$

These approximate solutions were in very close agreement with the maximum and minimum values for 2V obtained by allowing α, β and γ to vary independently between the limits $\alpha \pm e\alpha$, $\beta \pm e\beta$ and $\gamma \pm e\gamma$.

A value of $\pm 10^\circ$ to 20° is common and $\pm 30^\circ$ not impossible in the calculated range for 2V. The resultant types of errors found in the optical data are listed in column A Table 4.4. Optical data with errors of types 2,3,4,5,6, was checked carefully with the original source and corrected. The resultant distribution, free from transcription errors, is given in Column B. Apart from errors of type 2 (Banno 1964, table 7, spec. no. 3) and type 3 (Mathias 1952, p. 15), which represent impossible refractive index combinations in a biaxial mineral, it can be seen that a considerable number of published optical determinations are internally inconsistent. The discovery of inconsistencies in optical data is not new, for example Larsen & Berman (1934) and Layton (1965) have stressed the importance of checks of this type on optical data. To be fair many of the type

Table 4.4. Results of data validification on relation OPTICS.

Condition	A Before correction.	B After correction.
1. Either α, β, γ or 2V not determined.	678	679
2. Either $\alpha = \beta$, $\alpha = \gamma$ or $\beta = \gamma$	1	1
3. Either $\alpha > \beta$, $\alpha > \gamma$ or $\beta > \gamma$	10	1
4. The observed 2V within the range of calculated 2V's but of wrong sign	37	33
5. The observed 2V outside the range of calculated 2V's and of wrong sign.	36	18
6. The observed 2V outside the range of calculated 2V's but of correct sign.	81	84
7. The observed 2V inside the range of calculated 2V's and of correct sign.	337	364
	total 1180	total 1180

4 errors are associated with the determination of the sign on material with high 2V. Even allowing for this the number of internal inconsistencies is disquietingly large.

The data in the amphibole data file has been used extensively in subsequent Chapters.

5. CLASSIFICATION OF THE AMPHIBOLES.

In this Chapter the relative merits of proposed projections and classifications of the calciferous and alkali amphiboles will be discussed (Section 5.1). The subdivision of amphibole compositional space will be reconsidered. An improved subdivision will be given and a method whereby a composition can be described in terms of a consistent combination of 'end members' will be discussed in Sections 5.2, and 5.3 respectively. The nomenclatural status of the 'end members' miyashiroite and sundiusite is discussed in Section 5.4. An extended amphibole compositional space capable of showing the major variation of all the amphiboles is described in Section 5.6 and the nomenclature of the required additional 'end members' is discussed.

5.1. Proposed graphical representations and classifications for the calciferous and alkali amphiboles.

Phillips' (1966) derivation of amphibole compositional space, Fig. 5.1, has been described in Chapter 1. Independently of Phillips, Fabries (1966) devised a topologically equivalent system for the calciferous and alkali amphiboles, Fig. 5.2a. Fabries made no attempt to name analyses falling in the derived space. Whittaker (1968) suggested a third topologically equivalent system, Fig. 5.2b, in which,

$$x = M^{2+} - \square \text{ in the X group,}$$
$$y = M^{3+} + 2M^{4+} - M^{+} - 2\square \text{ in the Y group,}$$
$$z = Si^{4+} + \square - 6 \text{ in the Z group.}$$

Each co-ordinate represents the increase in charge above the minimum and the space so defined was termed 'charge distribution space'. Orthorhombic and cummingtonite amphiboles can also be included, while oxyamphiboles may lie outside the space. Whittaker subdivided charge distribution space and adjacent space into a number of named and unnamed cubic cells.

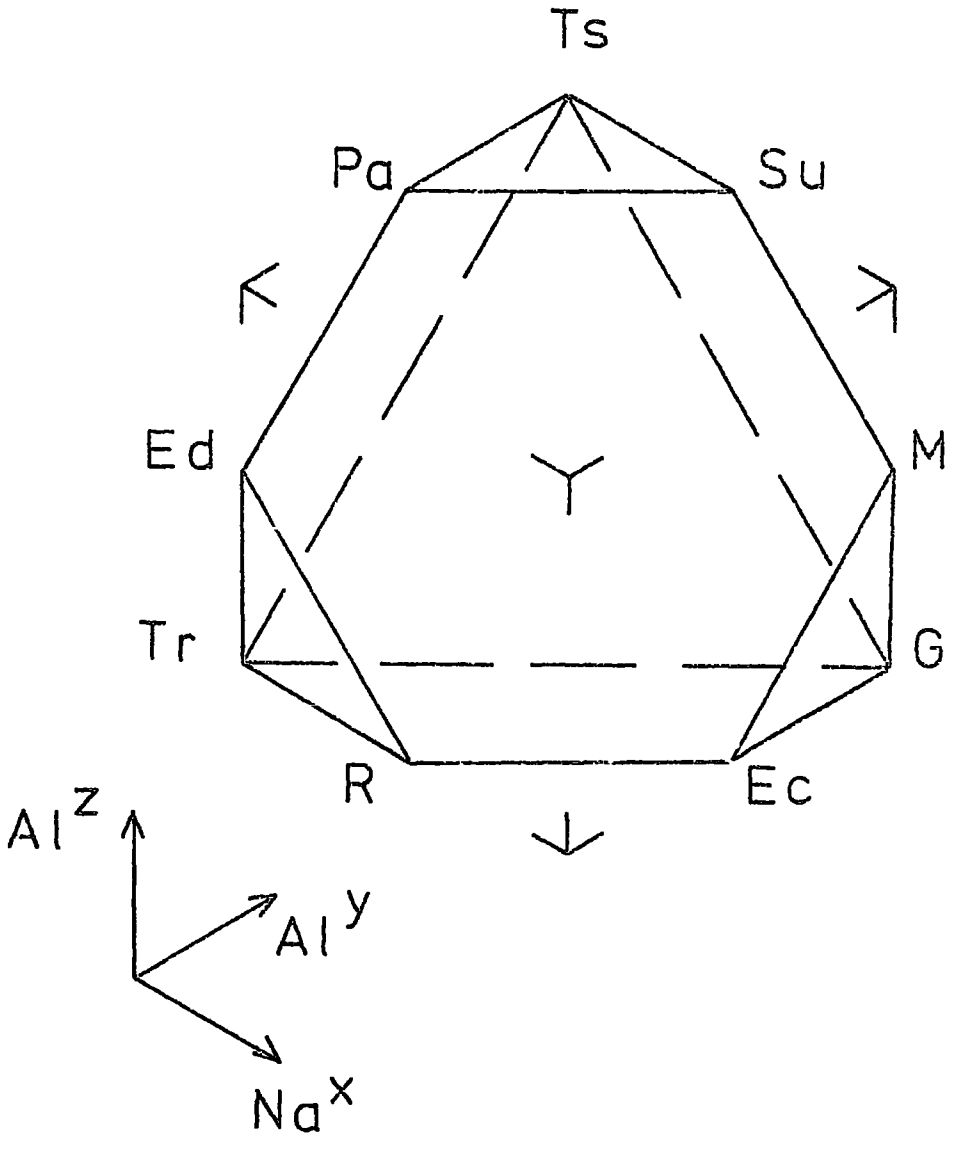


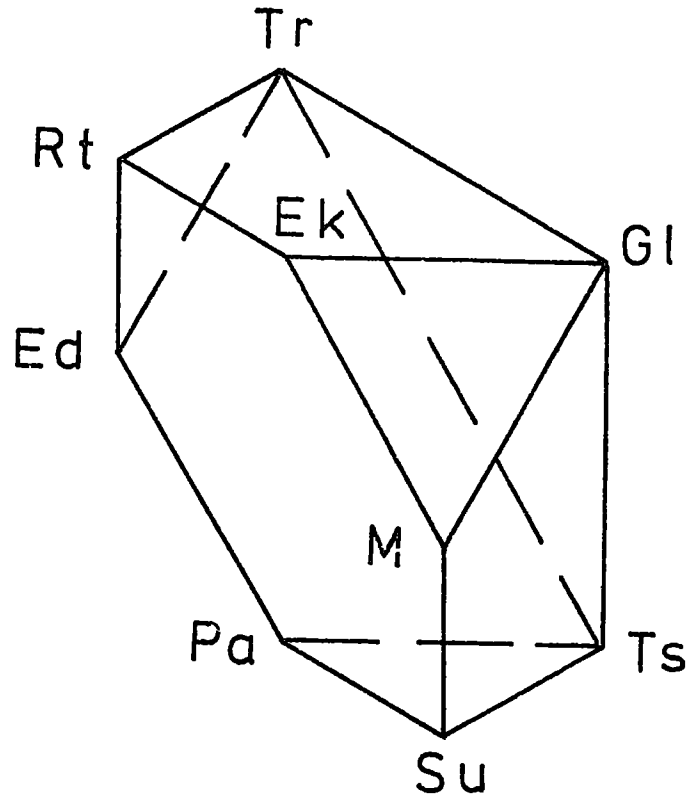
Fig 5.1. Amphibole compositional space after Phillips (1966). Abbreviations are as follows :- Tr tremolite, Ts tschermakite, G glaucophane, Ed edenite, Pa pargasite, Su sundiusite, M miyashiroite, Ec eckermannite and R richterite.

Fig. 5.2. Graphical representations of the calciferous and alkali amphiboles after Fabries (1966) and Whittaker (1968).

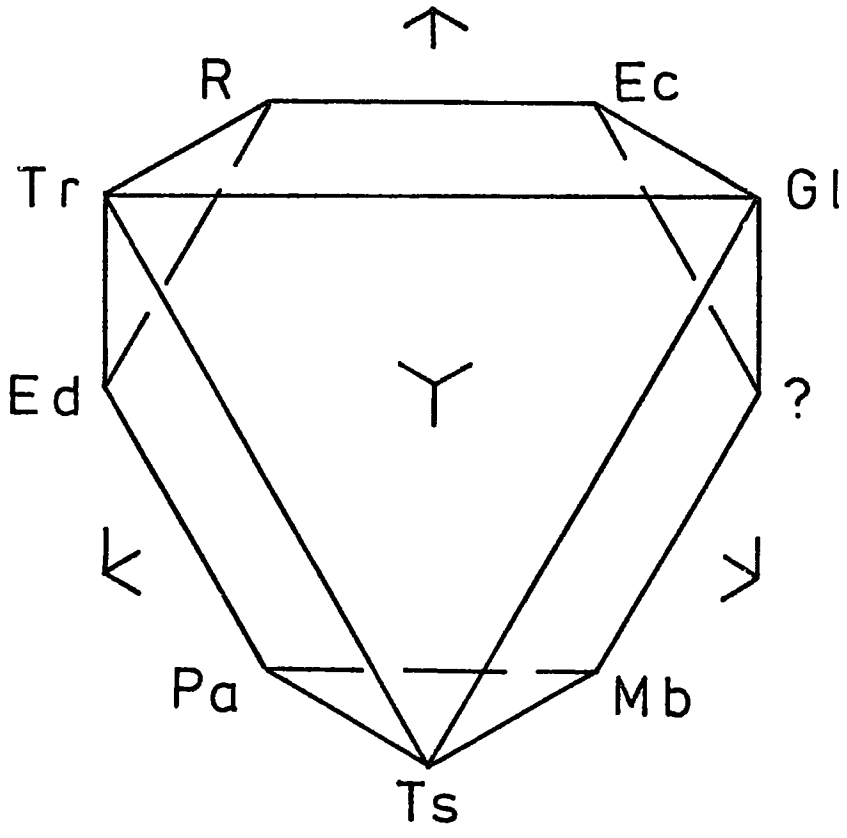
(a) Space occupied by calciferous and alkali amphiboles after Fabries (1966). Abbreviations are the same as in Fig. 5.1 with the following exceptions: - Gl glaucophane, Ek eckermannite and Rt richterite.

(b) Charge distribution space after Whittaker (1968). Abbreviations are as Fig. 5.1 with the following exceptions: - Mb mboziite in place of sundiusite and (?) in place of miyashiroite.

a



b



The systems of Phillips and Whittaker both have many points in common and it is of interest to discuss the relative merits of the two systems at this point. Provided there are no uncompensated vacancies in the X and Y groups the two systems are related by

Whittaker	Phillips
x	$2 - Na^X$
y	Al^Y
z	$2 - Al^Z$

At first sight the Phillips system appears inferior in two aspects. Firstly orthorhombic and cummingtonite amphiboles are not included and secondly the possibility that isomers of certain compositions, for example richterite, may plot outside amphibole compositional space.

The conceptsof the basic atomic formula and amphibole compositional space were originally defined for calciferous and alkali amphiboles. Orthorhombic and cummingtonite amphiboles can be included if (Mg^{2+}, Mn^{2+}, Fe^{2+}) and Li^+ in the X group are included with Ca and Na^X respectively and any Li^+ in the A group (protoamphibole) as Na^A, in the calculation of the basic atomic formula. Anthophyllite $\square Mg^{2+}_2Mg^{2+}_5Si^{4+}_8O^{2-}_{22}(OH^-)_2$, gedrite $\square Mg^{2+}_2Mg^{2+}_3Al^{3+}_2Si^{4+}_6Al^{3+}_2O^{2-}_{22}(OH^-)_2$ and holmquistite $\square Li^+_2Mg^{2+}_3Al^{3+}_2Si^{4+}_8O^{2-}_{22}(OH^-)_2$ plot as tremolite, tschermakite and glaucophane respectively in both systems.

Whittaker (1968, p.238) introduced the possibility of positional isomerism of Na^+ and Ca^{2+} between the A and X groups in compositions such as richterite $Na^+Ca^{2+}Na^+Mg^{2+}_5Si^{4+}_8O^{2-}_{22}(OH^-)_2$ and 'iso-richterite' $Ca^{2+}Na^+_2Mg^{2+}_5Si^{4+}_8O^{2-}_{22}(OH^-)_2$. Iso-richterite would plot outside amphibole compositional space. A study of the Madelung energies of richterite and 'iso-richterite' by Whittaker (1971) demonstrated that richterite was the lower energy isomer.

X-ray refinement of the crystal structure of two synthetic richterites by Cameron & Gibbs (1971), in which all Ca^{2+} was arbitrarily ordered into the X group, yielded low residual 'R factors' indicating that the ordering used was probably correct. Natural compositions may be expected to have Na^{+} and not Ca^{2+} in the A group. This is in accordance with Phillips (1963) and the calculation of atomic formulae in Chapter 2. There would appear to be no evidence, at least at present, to require amphibole compositional space to be extended in this respect.

The Phillips system may be considered superior in two aspects, the treatment of oxyamphiboles and 'real' compositions subject to analytical error. According to Phillips (1963) oxygens substituting for hydroxyls are balanced by ferric iron in the Y group ($Fe^{2+} + OH^{-} = Fe^{3+} + O^{2-}$), although the validity of this substitution has been questioned by Leake (1968). The resultant ferrous iron is returned as Mg in the basic atomic formula. In this way oxyamphiboles plot within amphibole compositional space nearest the end member they are most similar to. Thus for example, an oxyhastingsite $Na^{+}Ca^{2+}{}_{2}Fe^{2+}{}_{3}Fe^{3+}{}_{2}Si^{4+}{}_{6}Al^{3+}{}_{2}O^{2-}{}_{22}(OH^{-},O^{2-})_{2}$ would plot as Pa and an oxyriebeckite $\square Na^{+}{}_{2}Fe^{2+}{}_{2}Fe^{3+}{}_{3}Si^{4+}{}_{8}O^{2-}{}_{22}(OH^{-},O^{2-})_{2}$ would plot as G. The same two compositions according to Whittaker have the co-ordinates 2,2,0 and 0,3,2 and plot as Ts and outside charge distribution space respectively. The overall relationship of the oxyamphibole is not as apparent as offered by Phillips' method. Secondly, when considering 'real' compositions it is apparent that negative co-ordinates are possible in the Whittaker system if Si^{4+} is less than 6.0 and possibly also for the X and Y axes if there are uncompensated vacancies in either group. In summary, of the two alternative systems, that proposed by Phillips is superior.

A number of other graphical representations and classifications have been suggested for specific groups of amphiboles. Many of these may be considered as views of portions of amphibole compositional space. The essentially similar plots for the calciferous amphiboles proposed by Hallimond (1943), Winchell (1945) and Boyd (1959) are projections onto the quadrilateral Tr - Ed - Pa - Ts of analyses with low Na^X. Leake (1968) has proposed a classification of the calciferous ($Ca^{2+} > 1.5$) and subcalciferous ($1.0 < Ca^{2+} < 1.5$) amphiboles in terms of a plot of Si^{4+} versus $Na^+ + Ca^{2+} + K^+$ (site unspecified). The ratio $Mg^{2+}/(Fe^{3+} + Fe^{2+} + Mn^{2+} + Mg^{2+})$ was erected perpendicular to the base. The space so defined was subdivided into a number of cells in such a manner as to maintain, as far as possible, the traditional use of nomenclature. In Fig. 5.3 the relationship between calciferous and subcalciferous amphiboles and the planes Tr - Ed - Pa - Ts and Tr - Ed - R representing Leake's projection is indicated. The major disadvantages of the system lie in the choice of the three variables used to define the name. In particular the occupancy of the Y group is not indicated directly and all compositions with the same (value for) Al^{iv} in the Z group and A site occupancy plot as the same point, see Fig. 5.3.

The most frequently used classification of the alkali amphiboles is that of Miyashiro (1957). This may be considered a projection of alkali amphiboles ($Na^X > 1.0$) onto the face $Na^X = 2.0$ in Fig. 5.1.

It is apparent from the above discussion that amphibole compositional space offers a convenient means of representing graphically the complex crystal chemistry of the calciferous and alkali amphiboles.

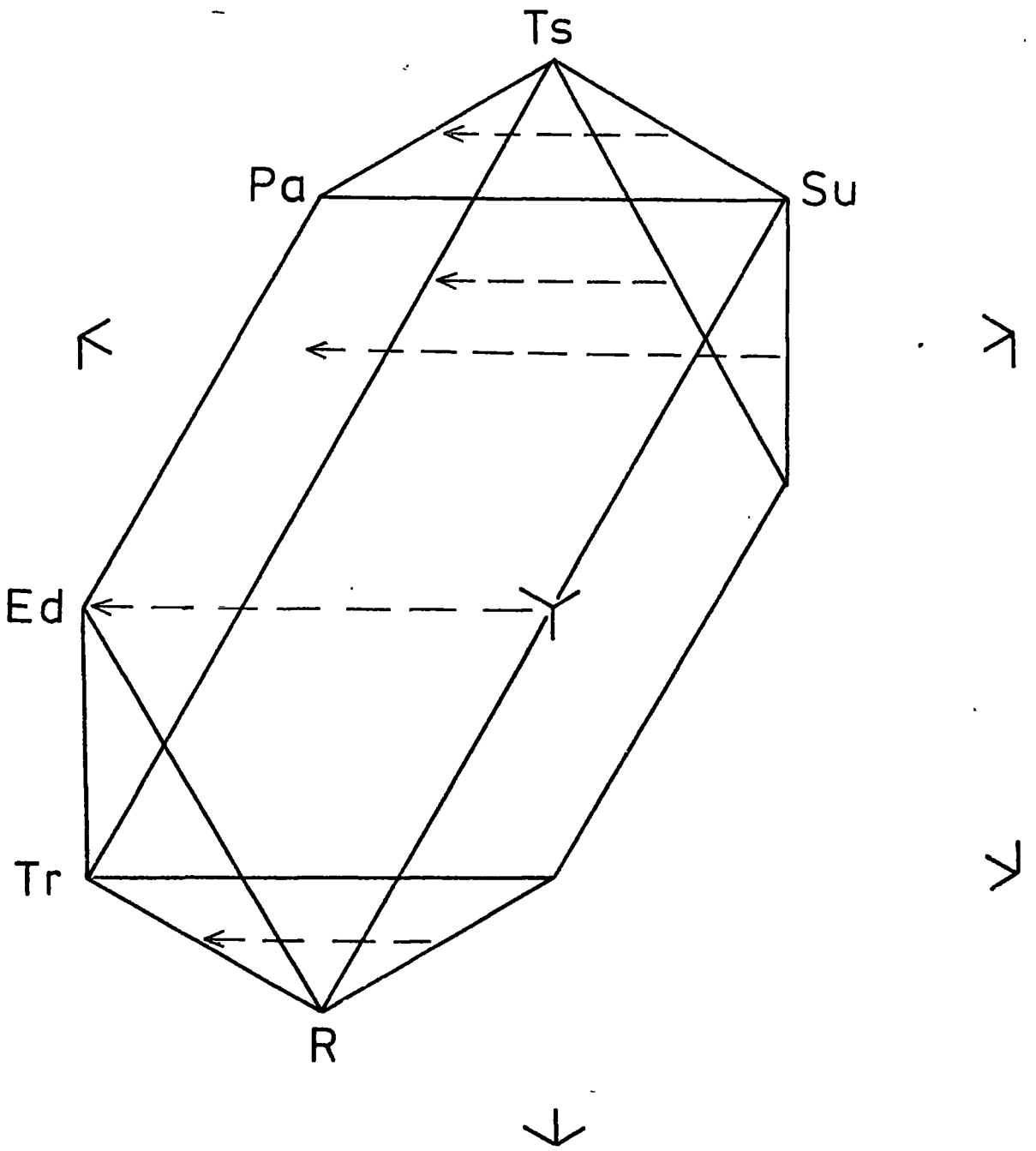


Fig. 5.3. The scope of analyses which project onto Leake's (1968) graphical representation of the calciferous and subcalciferous amphiboles. All compositions along the length of each arrow, that is with the same Al^Z and Na^A, project as the same point on the planes Tr - Ed - Pa - Ts and Tr - Ed - R.

5.2. Subdivision and nomenclature of amphibole compositional space.

Whittaker (1968) suggested that charge distribution space could be subdivided into a number of cubic cells, each centred about an integral co-ordinate and extending $\pm$ 0.5 units along the x, y and z axes. Applying the same scheme to amphibole compositional space requires 19 cells. These include 9 centred about each of the 'end members', 3 more at the mid-points of the edges of the triangular face Tr - Ts - G and 1 at the centre of the hexagonal face. The remaining 6 are centred outside compositional space at 1,2,0; 0,1,0; 0,2,1; 2,1,1; 1,0,1; and 1,1,2 (Phillips co-ordinates). Each cell can be identified by the co-ordinates of the central point or named after characteristic amphiboles plotting within the cell. An unknown can be identified simply, but the requirement of such a large number of cells is in the writers opinion prohibitive. In addition the proportion of individual cells within amphibole compositional space varies considerably.

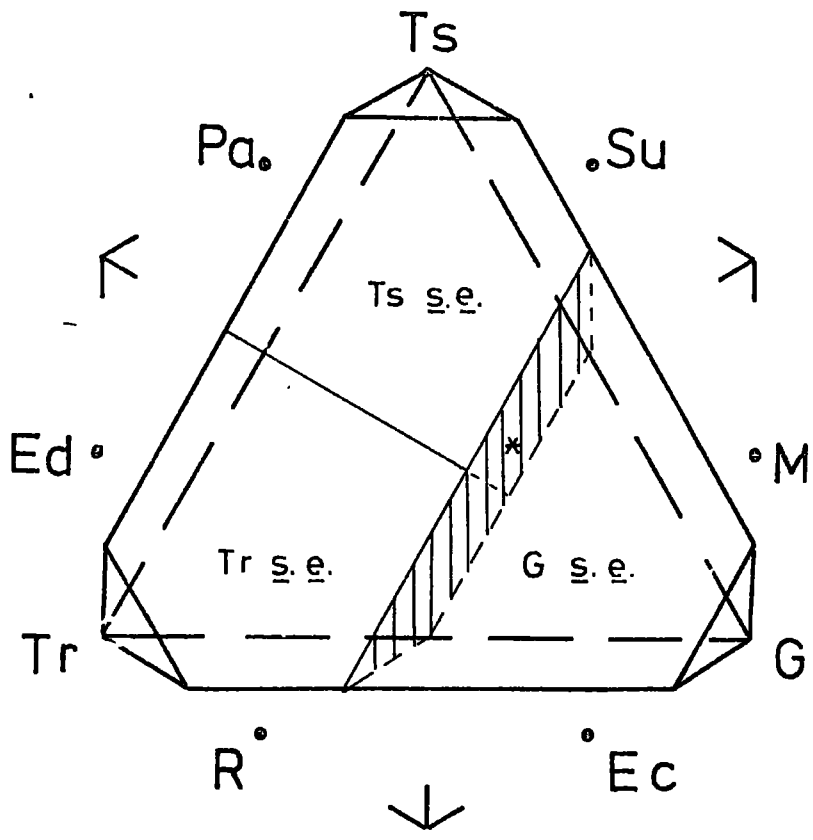
Phillips & Layton (1964) suggested the term sensu extenso to characterise compositions with greater than 50 per cent of a specific 'end member' present. Phillips (1966) subdivided amphibole compositional space into 'sensu extenso' regions. The apostrophes have been included to indicate that the regions given by Phillips do not correspond throughout with greater than 50 per cent of 'end members'. For example, Phillips subdivision of compositions with $Na_A < 0.5$ is given in Fig. 5.4a and compared with regions in which 'end members' are each in excess of 50 per cent in Fig. 5.4b. Further examination of Fig. 5.4a reveals that the three 'sensu extenso' regions do not correspond with regions in which a specific 'end member' even predominates. A composition such as $\square Ca^{2+}_{1.1}Na^{+}_{0.9}Mg^{2+}_{3.5}Al^{3+}_{1.5}Si^{4+}_{7.4}Al^{3+}_{0.6}O^{2-}_{22}(OH^{-})_2$, marked (米)

Fig. 5.4. Subdivision of amphibole compositional space with $Na^{A} < 0.5$.

(a) 'Sensu extenso' regions after Phillips (1966).

(b) Subdivision into regions in which each of the 'end members' accounts for greater than 50 per cent of the compositional variation. Three regions each with the same shape as amphibole compositional space correspond with sensu extenso regions in the original sense. The central region and three peripheral tetrahedral regions do not correspond to greater than 50 per cent of any 'end member'.

a



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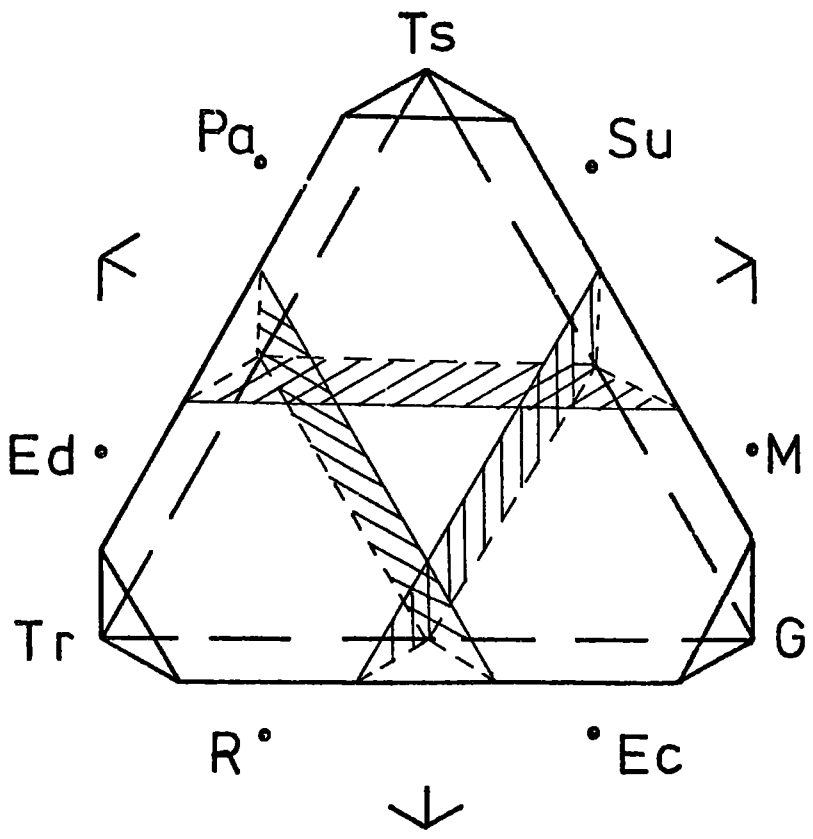


in Fig. 5.4a, and lying in the field of Ts '*sensu extenso*' is represented by the 'end member' combination $Ts_{30}G_{45}Tr_{25}$! .

Amphibole compositional space with $Na^A > 0.5$ is shown in Fig. 5.5. Regions with greater than 50 per cent of a specific 'end member' present are overlapping, (Fig. 5.5b). Three tetrahedral regions, stippled in Fig. 5.5b, cannot be described in terms of greater than 50 per cent of any of the available 'end members'. The '*sensu extenso*' nomenclature of Phillips, Fig. 5.5a, corresponds in this case with regions in which 'end members' predominate only.

To the writer the subdivision of amphibole compositional space into regions in which 'end members' either predominate or are in excess of 50 per cent offers an obvious way of naming amphiboles without extending the number of names required unnecessarily. If the space is to be subdivided into regions which can be described by greater than 50 per cent of a composition a number of additional 'end members' are required. However, amphibole compositional space can be subdivided into regions in which the nine 'end members' dominate without the addition of any further names. These regions are indicated in Fig. 5,6a,b and the name *sensu dominante* (abbreviated to *s.d.*) is suggested to distinguish these from *sensu extenso* regions. A *sensu dominante* name can be obtained by consulting Table 5.1.

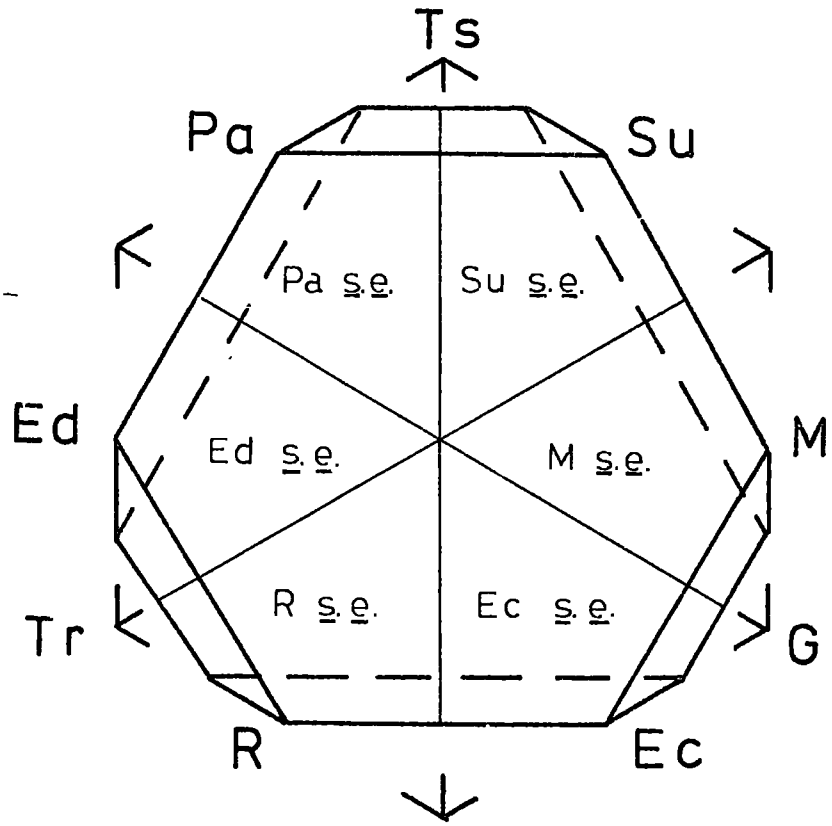
The advantage of such a subdivision lies in its ability to name an analysis in accordance with the dominant 'end member' component of the basic atomic formula. The boundaries are parallel for compositions with $Na^A < 0.5$ and $Na^A > 0.5$ which was not so in the original subdivision. The major disadvantage of the proposed subdivision is that Phillips' (1966) boundary ($Na^X = 1$) separating the calciferous and alkali amphiboles no longer corresponds with that between *sensu dominante* names. However any large scale boundary which is based on only a single variable (Na^X) is in many ways less

Fig. 5.5. Subdivision of amphibole compositional space with $Na > 0.5$.

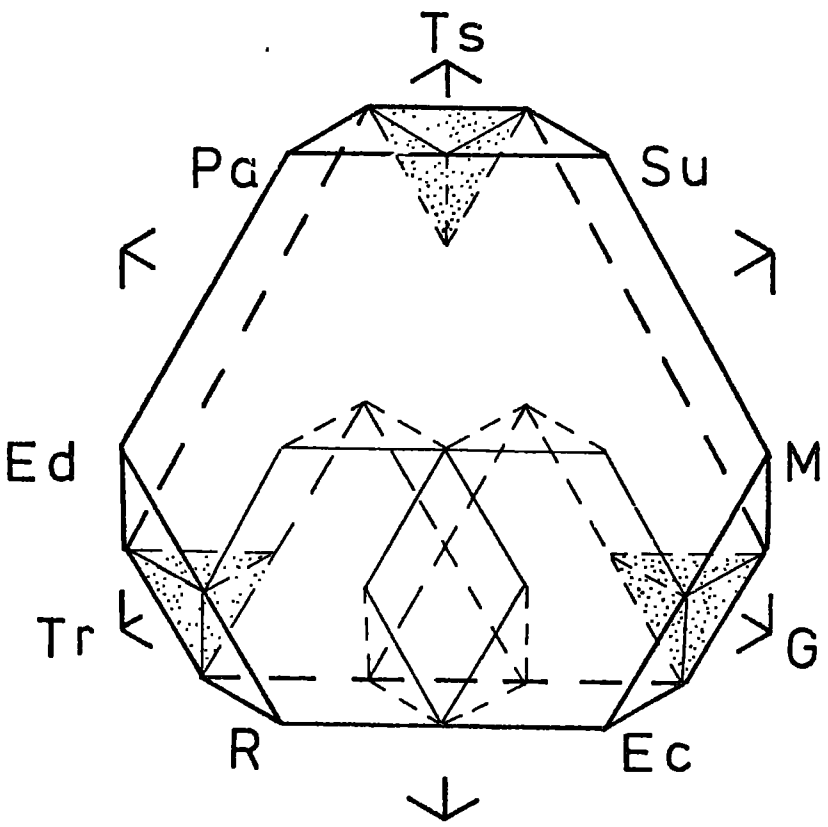
(a) '*Sensu extenso*' regions after Phillips (1966). The three boundary planes are parallel to the line of sight in this diagram.

(b) Subdivision into regions in which each of the 'end members' accounts for greater than 50 per cent of the compositional variation. Only two of the six overlapping true *sensu extenso* regions are shown, those corresponding to R *sensu extenso* and Ec *sensu extenso*. Three tetrahedral regions, stippled, do not correspond to greater than 50 per cent of any of the 'end members'.

a


Ts
Pa
Su
Pa s.e.
Su s.e.
Ed
M
Ed s.e.
M s.e.
Tr
G
R s.e.
Ec s.e.
R
Ec

b


Ts
Pa
Su
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M
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Ec

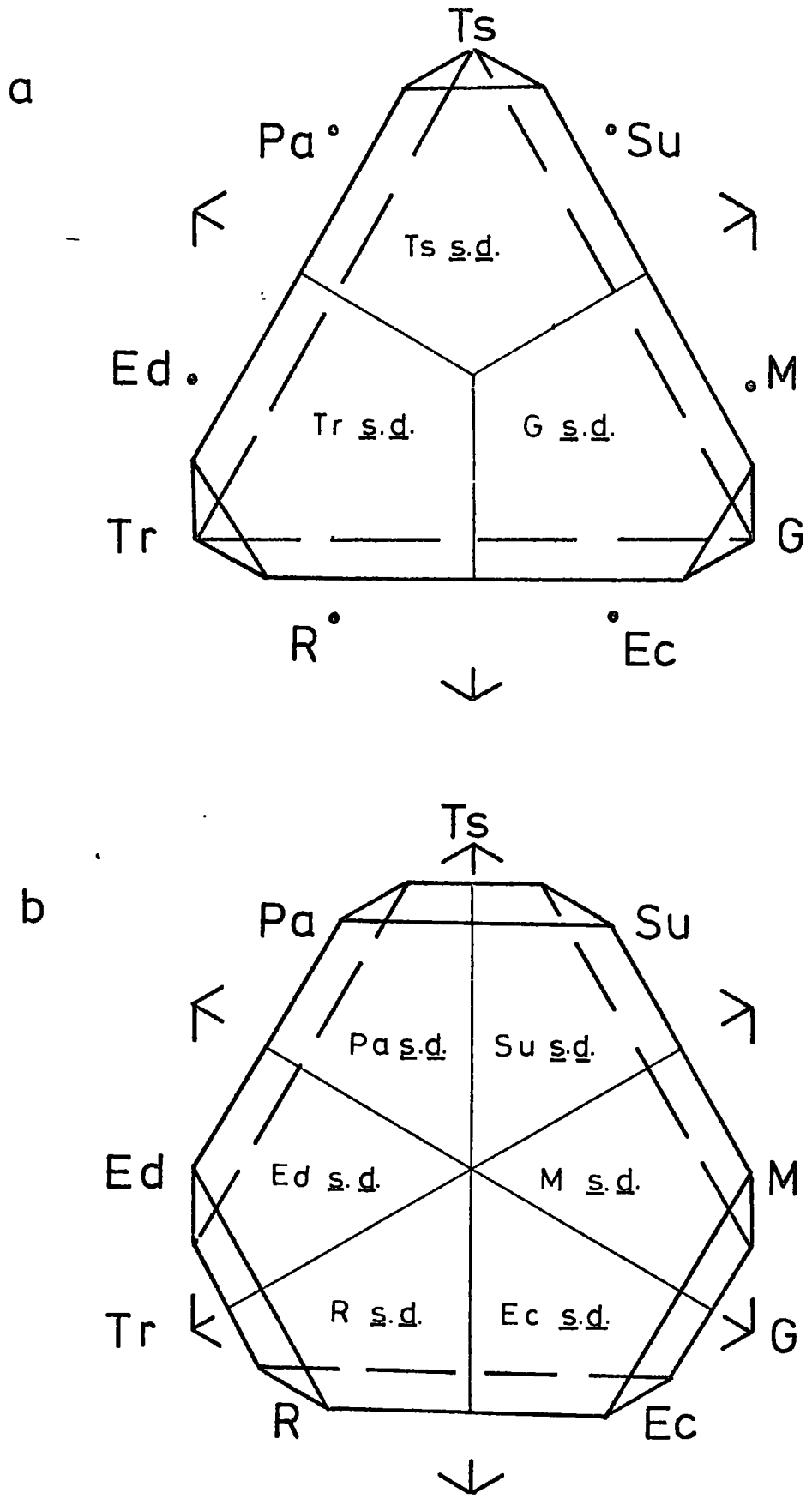

Fig.5.6. Proposed subdivision of amphibole compositional space into sensu dominante regions.

(a) $Na^A < 0.5$, (b) $Na^A > 0.5$.

Table 5.1. Determination of the sensu dominante name.

Al^Y	Al^Z	Unique	Special	A	B	C	D	etc
X = 0.05								
0-0.5	0-0.5	-	-	Tr	R	-	-	Ed
	>0.5-1.0	-	-	Tr	-	-	-	Ed
	>1.0-1.5	Ed	-	-	-	-	-	
.5-1.0	0-0.5	Tr	-	-	-	-	-	
	> 0.5-1.0	-	-	Tr	-	-	-	Ed
	> 1.0-1.5	-	A + C Tr	Ts	-	Ed	-	Pa
	> 1.5-2.0	Pa	-	-	-	-	-	
.0-1.5	> 0.5-1.0	-	A + C Tr	-	-	-	-	Ts
	> 1.0-1.5	-	-	Ts	-	-	-	Pa
	>1.5-2.0	-	-	Ts	-	-	-	Pa
5-2.0	>1.0-1.5	Ts	-	-	-	-	-	
	1.5-2.0	-	-	Ts	-	-	Pa	Sa
= >0.5-1.0								
-0.5	0-0.5	-	-	Tr	-	-	-	R
	>0.5-1.0	-	-	-	R	-	-	Ed
.5-1.0	0-0.5	-	-	Tr	-	-	-	R
	>0.5-1.0	-	-	Tr	R	-	-	Ed
	>1.0-1.5	-	-	-	-	Ed	-	Pa
.0-1.5	0-0.5	-	A + D Tr	-	-	-	-	G
	>0.5-1.0	-	A+C+D Tr	-	-	-	-	
		-	A + B G	Ts	-	-	-	
		-	B + D R	-	-	-	-	
		-	C + D Ed	-	-	-	-	
		-	C + B Ec	-	M	-	Pa	Su
	>1.0-1.5	-	-	Ts	-	-	Pa	Su
	>1.5-2.0	-	-	-	-	-	Pa	Su

>1.5-2.0	0.5-1.0	-	A + B	G	Ts	-	-	-
	1.0-2.0	-		-	Ts	-	-	- Su
		-		-	-	-	-	-
Na^X 1.0-1.5								
0-0.5	0-0.5	R		-	-	-	-	-
0.5-1.0	0-0.5	-	A + D	Tr	G	-	-	R Ec
	>0.5-1.0	-		-	-	-	-	R Ec
1.0-1.5	0-0.5	-		-	G	-	-	- Ec
	>0.5-1.0	-		-	G	-	Ec	- M
	>1.0-1.5	-		-	-	M	-	- Su
1.5-2.0	0-0.5	G		-	-	-	-	-
	>0.5-1.0	-		-	G	-	-	- M
	>1.0-1.5	-	A + B	G	Ts	M	-	- Su
	1.5-2.0	Su		-	-	-	-	-
Na^X >1.5-2.0								
0.5-1.0	0-0.5	Ec		-	-	-	-	-
1.0-1.5	0-0.5	-		-	G	-	-	- Ec
	>0.5-1.0	-		-	-	-	Ec	- M
1.5-2.0	0-0.5	-		-	G	-	Ec	- M
	>0.5-1.0	-		-	G	-	-	- M
	>1.0-1.5	-		-	-	-	-	- M

Conditions

A $Al^Z \leqslant Al^Y - Na^X + \frac{1}{2}$

B $Al^Z \leqslant Na^X$

C $Al^Z \leqslant {}^{2-} Al^Y$

D $Al^Y \leqslant {}^{2-} Na^X$

informative than a nomenclature based on the dominant component of the basic atomic formula. The question of subdividing amphibole compositional space in terms of Na^X is returned to in Chapter 7 after examining the distribution of natural amphiboles.

5.3. Derivation of consistent 'end member' combinations for basic atomic formulae in amphibole compositional space.

There are instances when a description of an analysis in terms of a linear combination of 'end members' is advantageous, as for example in the study of the optical properties of amphiboles along a join between two 'end members'. Compositions within amphibole compositional space can be described as a linear combination of the vertices but for other than special instances (vertices) more than one combination of 'end members' is possible, (see Chapter 1). A simple method is outlined below by which the most appropriate 'end member' combination can be arrived at consistently.

Knowing the sensu dominante name for an analysis it is logical to derive an 'end member' combination in which the sensu dominante component is a maximum. Often this single restriction is enough to provide a unique combination. If an analysis can be described by a number of combinations in which the sensu dominante component is equally important it is suggested that the combination involving the smallest number of 'end members' is chosen. Where this is still not unique then the combination involving the smallest number of 'end members' to account for the highest proportion of the composition is used. This is best illustrated by a formal description of the method and some actual examples.

1) Calculate a basic atomic formula from the analysis.

2) Check that the analysis lies within amphibole compositional space, $Al^Z \geqslant Al^Y - Na^X$, $Al^Z \leqslant Al^Y - Na^X + 1$, $Al^Z \leqslant 2.0$, $Al^Y \leqslant 2.0$,

$Na^X \leqslant 2.0$, $Na^A \leqslant 1.0$ and that $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$.

3) Determine one combination of 'end members' necessary to completely describe the basic atomic formula of the analysis. Normally this can be achieved by determining the maximum proportion of the sensu dominante component first (see Example 1). If this is not possible, as in the case of Tr sensu dominante (Example 2), it may be necessary to derive a combination by first determining the proportion of 'end members' other than the sensu dominante component.

5) Once an 'end member' combination has been calculated alternative combinations which also describe the analysis can be obtained with the aid of Table 5.2. In Table 5.2 pairs of 'end members' on each side of the equals sign have the same combined basic atomic formulae and are interchangeable. Thus a combination of Su_xR_y ($x > y$) becomes according to equivalence (1) $Ed_yM_ySu_{x-y}$ and a combination $Ec_xSu_yR_y$ from (2) becomes $Ec_{x+y}Pa_y$.

In determining the maximum proportion of the sensu dominante component start at the top of Table 5.2 and find all those equivalent combinations in which the required component does not decrease. Once an alternative has been obtained return to the top of the Table and check for any further alternatives to the combination. Continue in this way until all the alternatives have been exhausted.

6) Choose from the list of alternative combinations the one in which the sensu dominante component is a maximum, or if this is not unique the description, complete or partial, in terms of the smallest number of 'end members'.

Example 1. specimen number 759 (see Appendix 8 for literature source).

Su sensu dominante.

Determine the maximum sensu dominante component.

Table 5.2: Equivalent 'end member' combinations.

1	Su + R	=	Ed + M
2	Su + R	=	Pa + Ec
3	Ed + M	=	Pa + Ec
4	2Pa + R	=	2Ed + Su
5	2Su + Ed	=	2Pa + M
6	2R + Pa	=	2Ed + Ec
7	2R + M	=	2Ec + Ed
8	2M + R	=	2Ec + Su
9	2M + Pa	=	2Su + Ec
10	G + Ed	=	Tr + M
11	Tr + Su	=	Ts + R
12	G + Pa	=	Ts + Ec
13	Tr + 2Ec	=	G + 2R
14	Tr + 2M	=	Ts + 2Ec
15	Tr + 2Su	=	G + 2Pa
16	Ts + 2Ed	=	Tr + 2Pa
17	Ts + 2R	=	G + 2Ed
18	Ts + 2M	=	G + 2Su

Na^A	Ca	Na^X	Mg	Al^Y	Si	Al^Z	$O_{22}(OH)_2$	
0.61	1.43	0.57	3.29	1.71	6.25	1.75		
0.57	0.57	0.57	1.71	1.14	3.42	1.14		Su 57 per cent
0.04	0.86	-	1.58	0.57	2.83	0.61		

The only remaining 'end members' with a full A site are Ed and Pa. Arbitarily. Ed was chosen next.

0.04	0.08	-	0.20	-	0.28	0.04	Ed 4.0
-	0.78	-	1.38	0.57	2.55	0.57	
-	0.57	-	0.85	0.57	1.71	-	Ts 28.5
-	0.21	-	0.53	-	0.84	-	
-	0.21	-	0.53	-	0.84	-	Tr 10.5
-	-	-	-	-	-	-	

$Su_{57}Ts_{28.5}Tr_{10.5}Ed_4$

From Table 5.2 it can be seen that there is no more Su rich equivalent combination, and only one $Su_{57}Ts_{26.5}Tr_{12.5}Pa_4$ (equivalence 16) with an equal Su content. Of these two, the former is chosen because the higher proportion of the composition is represented by the smaller number of 'end members'.

Example 2, specimen number 910, Tr sensu dominante.

Here it is not possible to remove the maximum sensu dominante component first. The choice of the components used is arbitrary provided they comply with the basic atomic formula.

Na^A	Ca	Na^X	Mg	Al^Y	Si	Al^Z	$O_{22}(OH)_2$	
0.14	1.86	0.14	4.54	0.46	7.54	0.46		
0.14	0.14	0.14	0.42	0.28	0.84	0.28		Su 14 per cent
-	1.72	-	4.12	0.18	6.70	0.18		
-	0.18	-	0.27	0.18	0.54	0.18		Ts 9
-	1.54	-	3.85	-	6.16	-		
-	1.54	-	3.85	-	6.16	-		Tr 77
-	-	-	-	-	-	-		

$Tr_{77}Su_{14}Ts_9$

From Table 5.2 it can be seen that there are no alternative combinations with either an equal or greater Tr component.

Example 3, specimen number 1483, Ec *sensu dominante*.

This example is included to show that even if an initial combination in which the *sensu dominante* component is not dominant is obtained a combination in which it is dominant can be found with the aid of Table 5.2.

It should be noted that in this example it would have been possible to have removed the Ec component initially.

Na^A	Ca	Na^X	Mg	Al^Y	Si	Al^Z	$O_{22}(OH)_2$
0.91	0.55	1.45	4.31	0.69	7.86	0.14	
0.07	0.07	0.07	0.21	0.14	0.42	0.14	Su 7 per cent
0.84	0.48	1.38	4.10	0.55	7.44	-	
0.48	0.48	0.48	2.39	-	3.84	-	R 48
0.36	-	0.90	1.71	0.55	3.60	-	
0.36	-	0.72	1.44	0.36	2.88	-	Ec 36
-	-	0.18	0.27	0.19	0.72	-	
-	-	0.18	0.27	0.18	0.72	-	G 9
-	-	-	-	-	-	-	

$Ec_{36}Su_7R_{48}G_9$

From Table 5.2 the following alternative combinations are possible. Only these with Ec greater than 36 per cent are shown here.

(2) $Ec_{43}R_{41}G_9Pa_7$

(6) $Ec_{50}R_{27}G_9Ed_{14}$

(13) $Ec_{68}R_9Tr_9Ed_{14}$

(12) $Ec_{50}R_{41}G_2Ts_7$

(13) $Ec_{54}R_{37}Tr_2Ts_7$

(13) $Ec_{61}R_{23}Tr_9Pa_7$

(6) $Ec_{68}R_9Tr_9Ed_{14}$

The combination with maximum Ec is $Ec_{68}R_9Tr_9Ed_{14}$

Using Table 5.2 it has been shown how a combination in terms of the maximum sensu dominante name can be obtained. Obviously the same method can be applied to maximise any of the components should this be required. For example as part of a study of the optical properties of amphiboles on the join Tr - Pa, amphiboles with high Tr, Pa components would be required. These may be found by maximising the Tr and Pa components with the aid of Table 5.2. For example the composition $Ed_{60}Ts_{30}Tr_{10}$ in the field of Ed s.d. can be seen from equivalence (16) to lie on the Tr - Pa join at $Tr_{40}Pa_{60}$.

5.4 Nomenclatural status of miyashiroite and sundiusite.

In deriving the sensu dominante nomenclature for amphibole compositional space Phillips and Layton's (1964) nomenclature for the nine (Mg^{2+}, Al^{3+} substituted) 'end members' has been used. It can be argued that it is unjustified to name an 'end member' unless corresponding synthetic or natural amphiboles are known, or amphiboles occur with the 'end member' component dominant. Six of the 'end members' have been synthesised, Ts, Pa (Boyd 1959), G (Ernst 1961), Ed (Colville, Ernst & Gilbert 1966), R, Ec (Phillips & Rowbotham 1968). Attempts to synthesise Ts (Ernst 1968; Jasmund & Schafer 1972) and M, Su (Phillips & Rowbotham 1968) have proved unsuccessful. Moreover, Leake (1965a, 1971) failed to find any natural amphiboles close to tschermakite or ferro tschermakite and when Phillips and

Layton coined miyashiroite and sundiusite 'no minerals close to either composition were known to the authors'. Tschermakite, named by Winchell (1945) for a theoretical composition suggested by Hallimond (1943), is now in common use both for the original theoretical composition (Sundius 1946; Smith 1959; Colville, Ernst & Gilbert 1966; Ernst 1968) and for various ferrous ferric iron substituted analogues (Deer, Howie & Zussman 1963; Whittaker 1968). Sundiusite and miyashiroite have not met with such approval. Fleischer (1965) argued for the abolition of both terms on the grounds that no amphiboles were known, at that time, with either 'end members' as the dominant component.

In order to clarify the position as regards the terms miyashiroite and sundiusite, a search of the amphibole data file was undertaken for analyses with either M or Su as the dominant component.

5.4.1. Miyashiroite.

A search of the amphibole data file located six basic atomic formulae with M as the dominant component, five of which had M in excess of 50 per cent and therefore belong to M *sensu extenso* in its original sense. Atomic formulae to 23(O), and where appropriate 24(O), and brief descriptions of the occurrence, location and source of the analyses are given in Table 5.3. 'End member' combinations calculated in accordance with the rules given above are included. Where it has not been possible to derive an accurate 'end member' combination because the analysis lies outside amphibole compositional space, or has an unbalanced basic atomic formula, only the *sensu dominante* component is indicated.

Because of the unbalanced basic atomic formula of 2225 and the relatively small M component in 794 further attention is confined to the remaining four analyses. A plot of $Fe^{2+}/(Fe^{2+} + Mg^{2+})$ versus $Fe^{3+}/(Fe^{3+} + Al^{vi})$, Fig. 5.7, shows that the three

Table 5.3. Source and atomic formulae of amphiboles with M as the dominant component.

*794 ($M_{43}G_{38.5}Tr_{11.5}Ec_7$), Harker (1963), from a strongly foliated gneissic riebeckite granite, Carn Chuinneag, Scotland. A balanced basic atomic formula is achieved to 23(0) and 24(0).

*919 ($M_{69}Tr_{31}$) Holgate (1951) from a crossite quartz albite epidote sphene schist, Llanfairpwllgwyngyll, Anglesey. The analysed material is reported to have at most 1 per cent of epidote impurity. While charge balance is achieved in the basic atomic formula the OH^- content is very low and the Y group total (23(0)) is low.

1738 (M_{70}) Perchuk et al. (1967) albitised nepheline syenite, Dugda Massif, Tuva, USSR. No water was determined.

2158 (approx. $M_{76}G_{15}Ts_9$) Sutherland (1969) fenitized dacite or rhyclite, Mt. Homa, Kenya and occurs as late stage veins of amphibole after aegirine. The analysis was performed in duplicate by rapid wet chemical methods and judging from the atomic formula is satisfactory.

2225 (M_{51}) Velde (1971) late stage amphibole in a minette, St Helier, Jersey. The analysis is probably inferior since charge balance is not achieved using the 23(0) or 24(0) bases.

*2241 ($M_{72}Ec_9R_{12}Tr_7$) Volkov et al. (1962) amphibole lujavrite, Mt. Parguaiv, Lovozero complex. The analysis is apparently satisfactory.

In this and subsequent tables * signifies an amphibole which is included in Figs. 7.1-7.28, Chapter 7.

		794		919		1738	2158	2225		2241	
		23(O)	24(O)	23(O)	24(O)	23(O)	23(O)	23(O)	24(O)	23(O)	24(O)
Z	Si	7.57	7.55	7.31	7.44	7.24	7.02	7.41	7.45	7.28	7.24
	Al^{IV}	0.43	0.45	0.69	0.56	0.73	0.98	0.51	0.51	0.72	0.76
Y	Al^{VI}			0.64	0.80		0.19			0.17	0.12
	Ti	0.02			0.12	0.07	0.14	0.26	0.27	0.10	0.03
	Fe^{3+}	1.65	1.60	0.72	0.12	1.26	1.49	0.98	0.70	1.16	1.16
	Fe^{2+}	3.19	3.19	1.33	1.35	1.62	0.92	1.41	1.42	1.44	1.43
	Mg			1.60		1.74	2.29	2.23	2.35	1.34	1.33
	Mn					0.16				0.15	0.15
	Li									0.32	0.32
	Ti Mg	0.07	0.09	0.18	0.06	0.07		0.01			0.07
	Fe^{3+}Mg		0.01	0.06							
	Fe^{3+}(oxy)				0.85				0.29		
	Al Li									0.32	0.32
X	Ca	0.23	0.23	0.62	0.63	0.50	0.18	0.22	0.22	0.26	0.26
	Na	1.77	1.77	1.38	1.37	1.50	1.82	1.78	1.78	1.74	1.74
A	Na	0.07	0.07	0.60	0.65	0.63	0.70	0.78	0.80	0.66	0.64
	K	0.43	0.43	0.10	0.11	0.29	0.07	0.35	0.35	0.27	0.27
	H^+		0.13								0.25
OH	OH		1.50		1.15				1.71		1.07
	F		0.50								0.93
	O^{2-}				0.85				0.29		
	Na^A	0.50	0.62	0.70	0.75	0.92	0.76	1.13	1.15	0.93	1.17
	Al^Y	1.79	1.60	1.37	1.17	1.41	1.96	1.50	1.23	1.53	1.34
	Na^X	1.77	1.77	1.38	1.37	1.50	1.82	1.78	1.78	1.74	1.74
	Al^Z	0.43	0.45	0.69	0.56	0.73	0.98	0.51	0.51	0.72	0.76
$(Na^A+Al^Y)-(Na^X+Al^Z)$		0.00	0.00	0.00	-0.01	0.10	0.08	0.34	0.19	0.00	0.00

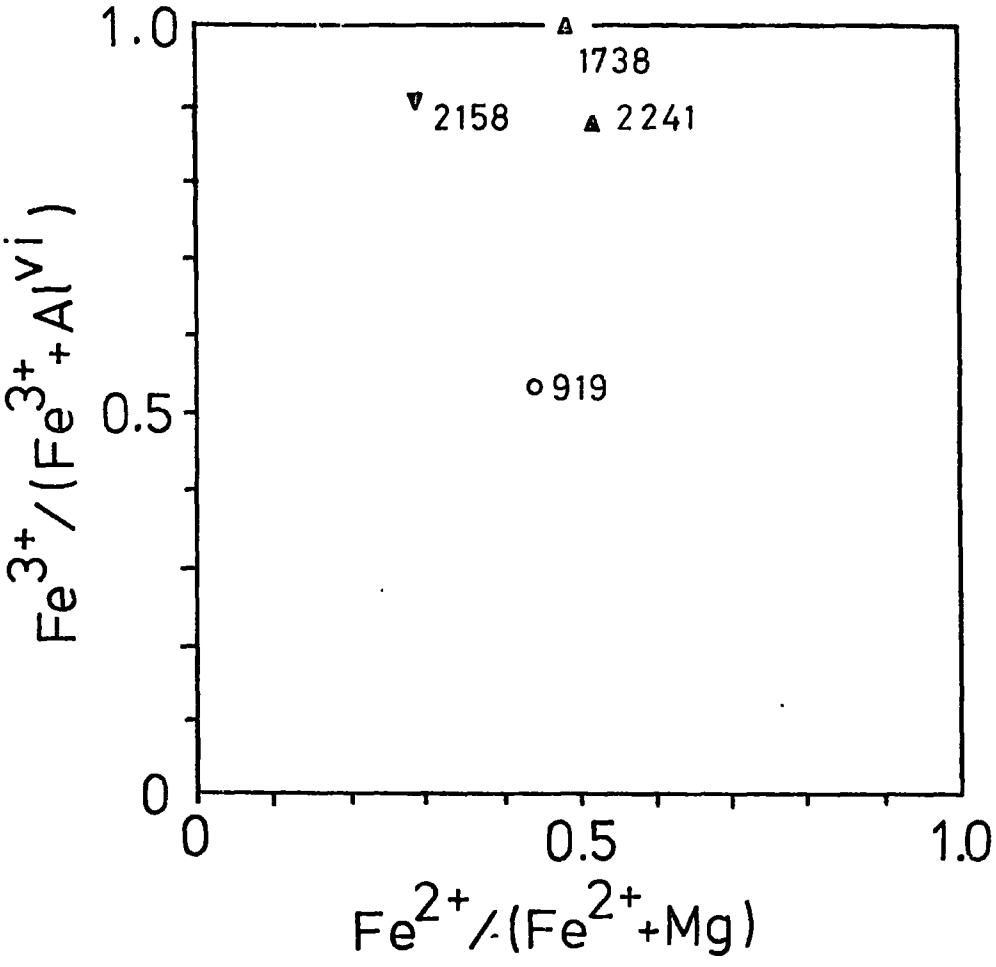

Fig. 5.7. $Fe^{2+}/(Fe^{2+} + Mg^{2+})$ and $Fe^{3+}/(Fe^{3+} + Al^{vi})$ in basic atomic formulae of amphiboles with the M component in excess of 50 per cent.

▲ alkali igneous host rock

▼ acid igneous host rock

o metamorphic host rock.

amphiboles from igneous parageneses are (Mg^{2+}, Fe^{2+}), Fe^{3+} substituted while the single amphibole from a metamorphic paragenesis is the most aluminous.

With the recognition of basic atomic formulae with $NaNa_2Mg_3Al_2Si_7AlO_{22}(OH)_2$ not only as the dominant component, but in excess of 50 per cent, there is, in the writers opinion, strong grounds for naming the component. Miyashiroite is the obvious name. Thus there are natural amphiboles with miyashiroite as the dominant component of the basic atomic formula but from Fig. 5.7 it is apparent that natural amphiboles close to the specific atomic formula $Na^{+}Na^{+}{}_2Mg^{2+}{}_3Al^{3+}{}_2Si^{4+}{}_7Al^{3+}O^{2-}_{22}(OH^{-})_2$ have still to be recognised. It is suggested that the name miyashiroite be retained for basic atomic formulae near $NaNa_2Mg_3Al_2Si_7AlO_{22}(OH)_2$ and possibly also for that specific composition. This is analogous with the modern use of tschermakite.

5.4.2. Sundiusite.

In the same year as sundiusite was first suggested Brock et al. (1964) described two amphiboles which approached the ferrous, ferric iron substituted analogue of sundiusite, $Na^{+}Ca^{2+}Na^{+}Fe^{2+}{}_3Fe^{3+}{}_2Si^{4+}{}_6Al^{2+}{}_2O^{2-}{}_{22}(OH^{-})_2$. These they termed mboziite after the Mbozi syenite - gabbro complex, Tanganyka where the type material was found. Fleischer (1965,1966) recognised mboziite as a valid amphibole name and Whittaker (1968) used it for the appropriate 'end member' of charge distribution space. Taking analyses from Deer, Howie & Zussman (1963) Whittaker found only a single amphibole plotted in cell 120 closest to mboziite. This was one of the type taramites of Morozewicz (1923) which like mboziite was ferrous, ferric iron rich.

A search of the amphibole data file for amphiboles with Su as the dominant component located 115 analyses. Many of these had only marginal Su dominance but 15 were found in which the Su component

was in excess of 50 per cent. Atomic formulae, location, occurrence and source of these which include the type taramite (280) and mboziite (1481) are given in Table 5.4. An optimum iron oxidation state has been estimated for the electron microprobe analysis 2719 and the extreme atomic formulae are given in Table 5.4.

Both the mboziites are apparently reliable analyses, however type taramite (1481) must be considered inferior. Ferrous iron substitution for Mg^{2+} and ferric iron for Al^{vi} can be seen from Fig. 5.8 where all fifteen analyses have been plotted. There is a marked concentration of analyses with ferrous and ferric iron substitution for Mg^{2+} and Al^{vi} which include the taramites and mboziites plus analyses 11, (Ainberg 1930), 82,83,87 (Appleyard in Leake 1968) and 940 (Holm 1971). Two of these latter analyses 82, 83 have 78 and 74 per cent Su component. It would appear that the ferrous, ferric iron substituted analogue of sundiusite, that is taramite or mboziite is not uncommon and occurs typically in nepheline bearing alkali igneous rocks and nepheline gneisses. Only two analyses, 844 (Heritsch & Kahler 1960) and 1413 (Machatchski & Walitzi 1963) do not show substantial Fe^{2+}, Fe^{3+} substitution.

The recognition of 115 basic atomic formulae with $NaCaNaMg_3Al_2Si_6Al_2O_{22}(OH)_2$ as the dominant component and fifteen in which it is in excess of 50 per cent are strong grounds for retaining the term sundiusite for such basic atomic formulae. The status of sundiusite is further strengthened by the recognition of analyses 844, 1413 both with the $NaCaNaMg_3Al_2Si_6Al_2O_{22}(OH)_2$ component equal to or greather than 50 per cent and with $Fe^{2+}/(Fe^{2+} + Mg^{2+})$ and $Fe^{3+}/(Fe^{3+} + Al^{vi})$ less than 0.5. It is possible that if such analyses had been recognised in 1964 when the term was first suggested, sundiusite might have met with general approval. The terms taramite or mboziite can be retained for the ferrous, ferric analogue of

Table 5.4. Source and atomic formulae of amphiboles with the Su component in excess of 50 per cent.

*11 ($Su_{59}Ed_{21}Ts_{20}$) Ainberg (1930), nepheline syenite, Ukraine, U.S.S.R. The OH^- content is very high.

*82 (Su_{78}), 83 (Su_{74}), 87 (Su_{55}) Appleyard in Leake (1968), nepheline gneiss, Kargus Ridge, Wolfe Belt, Lyndoch, Ontario.

*280 ($Su_{90}R_{10}$) Brock et al. (1964) type mboziite from late stage nepheline syenite dyke intruded into the Mbozi syenite - gabbro complex, Tanganyka.

*281 (approx. $Su_{70}Pa_{30}$) Brock et al. (1964), late stage pegmatitic nepheline syenite dyke intrusive into the Darkinale syenite complex, Somali Republic.

*424 ($Su_{53}Ts_{30}Tr_{17}$) Couyat (1908), andesite, Wadi Abu Maammel, Egypt. The analysis is an old one with Na_2O, K_2O expressed as Na_2O and the water content is probably in error.

*844 ($Su_{57}Ts_{29}Tr_{10}Ed_4$) Heritsch & Kahler (1960), vein in eclogite, Saulpe, Austria. The OH^- content is very high.

*940 Holm (1971, no. 3), leucocratic nepheline gneiss, Ghana. Despite the quoted high purity of the analysed material (>98%) and the use of wet chemistry the OH^- content is very low. When recalculated to 23(O) the analysis lies well outside amphibole compositional space so no 'end member' combination has been calculated.

*1403 (Su_{57}) Lupanova (1934), phenocrysts in a monchiquite dyke, Hibina Mts, Khibina Tundra U.S.S.R. The water content is loss on ignition and almost certainly in error.

*1413 ($Su_{50}Ts_{28}Tr_{22}$) Machatchski & Walitzi (1963), amphibolite, Stramez, Southern Koralpe, Austria. H_2O+ is assumed to make total up to 100.

1481 (Su_{51}) Morozewicz (1926) type taramite mariupolite dyke cutting

alkali granite, Mariupol, Ukraine, USSR. The analysis grossly fails to calculate to a balanced basic atomic formula.

*1482 (Su 68) Morozewicz (1926), as above. The water content is again too high.

*1667 (Su_{55}) Parsons (1930, no.1), the occurrence is not given. The water content is very low.

2719 ($Su_{64}Ts_{30}G_6$ to $Su_{70}Ts_{23}Tr_7$) Linthout & Kieft (1970), electron microprobe analysis of 'magnesium aluminium mboziite', schistose albitiferous quartzite, Sierra de los Filabries, Spain. The iron oxidation state has been estimated and lies between the values given in Table 5.4.

		* 11		* 82		* 83		* 87		* 280		* 281		* 424	
		23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)
Z	Si	6.22	6.04	5.94	5.97	5.95	5.98	5.78	5.82	6.19	6.20	5.98	5.98	6.34	6.55
	Al^{IV}	1.78	1.96	2.06	2.03	2.05	2.02	2.22	2.18	1.81	1.80	2.02	2.02	1.66	1.45
Y	Al^{VI}	0.28		0.29	0.33	0.24	0.28	0.42	0.48	0.14	0.15	0.36	0.36	0.45	0.72
	Ti	0.09				0.07	0.12	0.11	0.21	0.03	0.04				0.17
	Fe^{3+}	1.06	0.53	1.42	1.21	1.34	1.15	1.06	0.72	1.59	1.56	1.28	1.27	1.23	1.35
	Fe^{2+}	3.46	3.36	2.40	2.41	2.67	2.68	2.68	2.70	2.51	2.52	2.99	2.99	0.52	0.32
	Mg	0.13	0.12	0.36	0.36	0.34	0.34	0.39	0.40	0.30	0.30	0.20	0.20	2.36	2.44
	Mn			0.18	0.18	0.15	0.15	0.13	0.13	0.26	0.26				
Ti	Mg		0.09	0.16	0.11	0.09	0.04	0.10			0.08	0.04	0.04	0.16	
Fe^{3+}	Mg		0.27	0.01								0.04	0.03	0.04	
Fe^{3+}	(oxy)				0.23		0.19		0.35		0.03		0.01		
X	Fe^{2-}														0.22
	Ca	1.41	1.37	1.22	1.23	1.26	1.27	1.45	1.46	0.99	0.99	1.30	1.30	1.45	1.50
	Na	0.59	0.63	0.78	0.77	0.74	0.73	0.55	0.54	1.00	1.00	0.70	0.70	0.55	0.28
A	Na	0.37	0.30	0.64	0.66	0.57	0.58	0.58	0.60	0.46	0.46	0.50	0.50	0.53	0.83
	K	0.44	0.33	0.48	0.48	0.50	0.50	0.48	0.48	0.56	0.56	0.58	0.58		
	H^+		1.34												
OH	OH		2.00		1.38		1.43		1.31		1.78		1.99		0.49
	F				0.39		0.38		0.34		0.19				
	O^{2+}				0.23		0.19		0.35		0.03		0.01		
	Na^A	0.80	2.06	1.12	1.14	1.07	1.08	1.06	1.08	1.02	1.02	1.08	1.08	0.53	0.83
	Al^Y	1.52	0.53	1.71	1.66	1.72	1.67	1.71	1.63	1.80	1.79	1.64	1.63	1.68	2.41
	Na^X	0.59	0.63	0.78	0.77	0.74	0.73	0.55	0.54	1.00	1.00	0.70	0.70	0.55	0.28
	Al^Z	1.78	1.96	2.06	2.03	2.05	2.02	2.22	2.18	1.81	1.80	2.02	2.02	1.66	1.45
		-0.04	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01	0.01	0.00	0.00	-0.01	0.01	1.51

		844*		940*		1403*		1413*		1481		1482*		1667*		2719	
		23(O)	24(C)	23(C)	24(C)	23(C)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	23(C)
Z	Si	6.25	6.08	5.74	5.91	5.67	5.81	6.45	6.32	6.20	6.12	6.29	6.24	5.76	5.99	6.09	6.15
	Al^{IV}	1.75	1.92	2.26	2.09	2.33	2.19	1.55	1.68	1.65	1.63	1.71	1.75	2.24	2.01	1.91	1.85
Y	Al^{VI}	1.12	0.88	0.46	0.71	0.42	0.63	0.84	0.66					0.22	0.54	0.93	1.00
	Ti		0.10		0.16	0.45	0.46	0.12		0.09	0.09			0.32	0.62		0.06
	Fe^{3+}	0.50	0.48	1.95	1.06	0.77	0.79	0.47	0.16	1.42	1.40	1.36	1.39	1.32	1.37	1.11	0.72
	Fe^{2+}	0.89	0.87	1.18	1.22	0.21		1.01	0.99	3.21	3.17	3.03	3.01	0.86	0.68	1.67	2.02
	Mg	2.33	2.27	0.24	0.25	3.18	3.12	2.51	2.46	0.14	0.14	0.11	0.11	1.73	1.80	1.19	1.25
	Mn			0.14	0.14					0.15	0.23						
	TiMg	0.06		0.19	0.03			0.03	0.14			0.13	0.13	0.28		0.06	
	$Fe^{3+}Mg$			1.22					0.15			0.08	0.18				
	Fe^{3+}(oxy)				1.39												
X	Mn									0.09							
	Fe^{2+}						0.22								0.21		0.05
	Mg						0.15										
	Ca	1.43	1.39	0.90	0.93	1.43	1.47	1.50	1.47	1.40	1.38	1.19	1.18	1.41	1.46	1.24	1.25
	Na	0.57	0.61	1.09	1.07	0.57	0.17	0.50	0.53	0.51	0.62	0.81	0.82	0.59	0.32	0.76	0.70
A	Na	0.44	0.37	0.41	0.49	0.40	0.83	0.35	0.31	0.71	0.58	0.69	0.67	0.16	0.45	0.45	0.52
	K	0.17	0.17	0.54	0.56	0.35	0.36	0.15	0.15	0.44	0.44	0.47	0.46	0.39	0.41	0.19	0.18
	H^+		1.23						0.94		0.66		0.41				
OH	OH		2.00		0.61		0.82		2.00		2.00		2.00		0.22		
	O^{2-}				1.39												
	Na^A	0.61	1.77	0.96	1.05	0.75	1.19	0.50	1.39	1.15	1.61	1.15	1.54	0.55	0.86	0.64	0.70
	Al^Y	1.71	1.56	2.40	2.11	2.09	2.34	1.55	0.82	1.60	1.58	1.36	0.82	2.17	3.14	2.03	1.85
	Na^X	0.57	0.61	1.09	1.07	0.57	0.17	0.50	0.53	0.51	0.62	0.81	1.09	0.59	0.32	0.76	0.70
	Al^Z	1.75	1.92	2.26	2.09	2.33	2.19	1.55	1.68	1.65	1.63	1.71	1.75	2.24	2.01	1.91	1.85
		0.00	0.80	0.00	-0.01	-0.06	1.17	0.00	0.00	0.59	0.94	0.00	0.06	-0.09	1.65	[illegible]	[illegible]

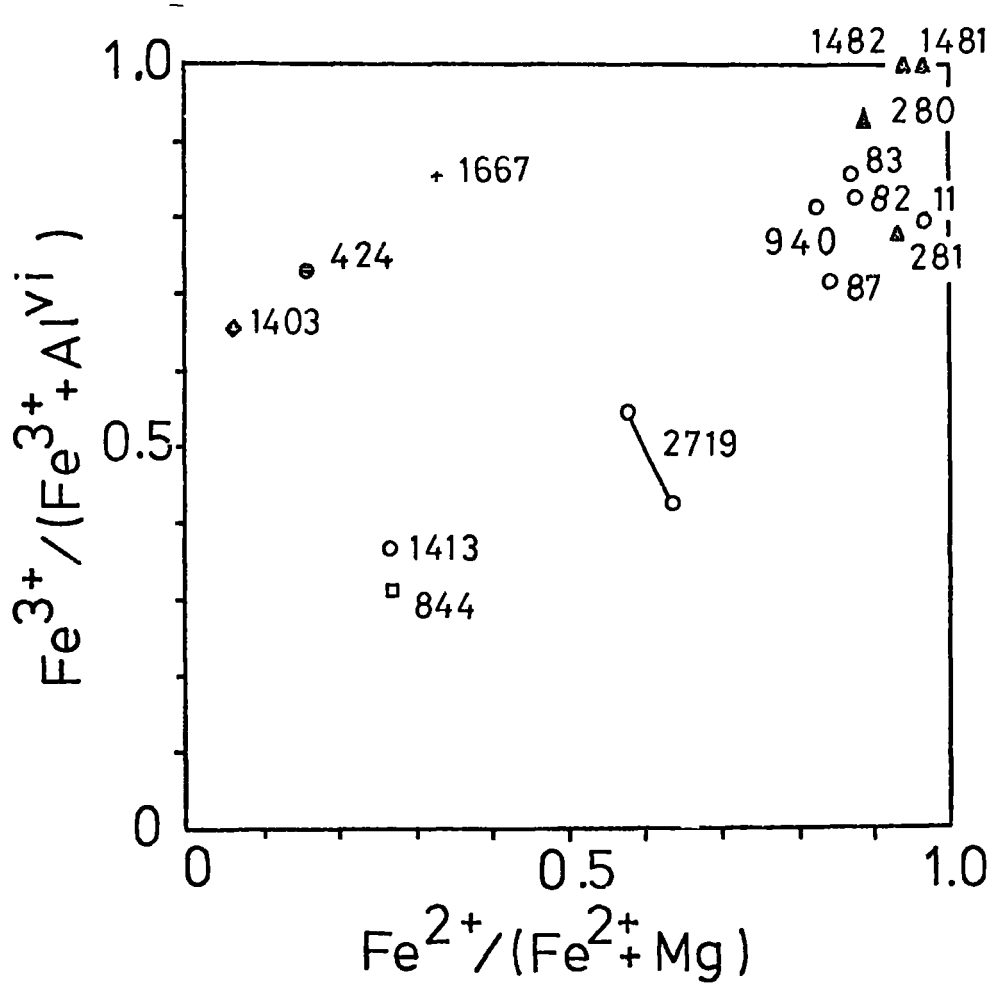

Fig. 5.8. $Fe^{2+}/(Fe^{2+} + Mg^{2+})$ and $Fe^{3+}/(Fe^{3+} + Al^{vi})$ in basic atomic formulae with the Su component in excess of 50 per cent.

- ● intermediate igneous host rock
- ▲ alkali igneous host rock
- ◆ basic alkali igneous host rock
- ○ metamorphic host rock
- □ eclogite host rock.

sundiusite.

5.5. Adjectival qualification of sensu dominante nomenclature.

The sensu dominante name along with the co-ordinates of the basic atomic formula are likely to be a satisfactory means of identifying, classifying and naming an amphibole for many purposes. However, the sensu dominante name does not indicate the extent of substitutions such as Fe^{2+} for Mg^{2+} and Fe^{3+} for Al^{vi} in the atomic formula both of which are ubiquitious and geologicaly important. This can be remedied by adding adjectival qualifiers to the sensu dominante name. It is suggested that the adjective ferro be used when Fe^{2+} excedes Mg^{2+} and ferri when Fe^{3+} excedes Al^{vi} in the atomic formula. Other substitutions such as K^{+} for Na^{+} in A (evidence presented in Chapter 2 suggested that K^{+} is confined to the A site) and Mn^{2+} for Mg^{2+} (this should be treated with caution since Mn^{2+} enters the X group when the sum of the Y group excedes 5.0) could also be treated in the same manner. Highly titaniferous amphiboles are a special problem and are considered below. An amphibole in Pa s.d. with Fe^{2+} in excess of Mg^{2+} and Fe^{3+} in excess of Al^{vi} can be described as ferro ferri pargasite (ferro ferri Pa s.d.).

A number of alternative names which are in common use for various ferrous, ferric iron substituted analogues of the 'end members' of amphibole compositional space are given below.

ferro Tr	ferroactinolite
ferri Pa	magnesiohastingsite
ferro ferri Pa	hastingsite
ferri G	magnesioriebeckite
ferro ferri G	riebeckite
ferri Ec	magnesioarfvedsonite (Andreev 1957)
ferro ferri Ec	arfvedsonite
ferro ferri Su	taramite (Morozewicz 1923), mboziite (Brock et al. 1964).

5.5.1. Kaersutite and highly titaniferous amphiboles.

The term kaersutite was introduced by Lorenzen (1884) for brown highly titaniferous amphibole from Kaersut, E. Greenland. The type material had a low hydroxyl content and this coupled with its colour led early workers to include all such amphiboles with the oxyamphiboles. Examination of small numbers of analyses by Wilkinson (1961) and Aoki (1963) showed that kaersutite represented titaniferous pargasite with limited substitution of Mg^{2+} by Fe^{2+} and a variable hydroxyl content. A similar conclusion was reached by Leake (1968) who with Aoki (1970) suggested that the lower titanium content should be 0.5 atoms. In view of the use and acceptance of kaersutite for a highly titaniferous amphibole it seemed worthwhile using the amphibole data file to outline the chemistry of amphiboles with Ti^{4+} in excess of 0.5 atoms and to consider the merit of kaersutite as an amphibole name.

A search of the entire amphibole data file for analyses with $Ti^{4+} \geqslant 0.5$ atoms to either 23(0) or 24(0) located 100 analyses (1). Since Wilkinson and Aoki showed that kaersutites had variable hydroxyl contents only those analyses with H_2O^+, F or Cl determined, Ca^{2+} in A less than 0.2 and total A site occupancy less than 1.1 atoms are included in Table 5.5. These latter criteria were added because Leake (1965a, 1971) has found that water determinations are frequently low. This will lead to an increased number of cations when calculated to 24(0) which tend to accumulate in the A site (cf Leake 1968, p. 18).

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(1) 35 * - 40, 42, 43, 45, 46, Aoki (1963); 34, Yagi (1953); 39, Harumoto (1933); 41, Kawano (1934); 56, 58, 59, Aoki (1970); 92, Bancroft & Howard (1923); 155, 159 - 163, Best (1970); 183, Adams (1903); 192, Binns (1969); 251 - 253, 255, 257, - 259, 262 - 265, 267, 268, Borley et al. (1971); 270 Bose (1963); 359, Campbell &

cont.

Table 5.5. Atomic formulae and basic atomic formulae of amphiboles with $Ti^{4+} \geqslant 0.5$ atoms.

		34		35		36*		37*		38*		39*		40*		41	
		23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)
Z	Si	6.04	6.04	6.00	6.07	5.80	5.94	5.68	5.80	5.75	5.88	5.73	5.87	5.71	5.82	5.65	5.75
	Al^{IV}	1.86	1.86	1.88	1.90	2.20	2.06	2.32	2.20	2.25	2.12	2.27	2.13	2.29	2.18	2.24	2.25
Y	Al^{VI}						0.20	0.44	0.62	0.28	0.47	0.11	0.31		0.16		0.06
	Ti	0.86	0.87	0.78	0.82	0.56	0.80	0.56	0.64	0.64	0.66	0.50	0.73	0.65	0.82	0.67	0.68
	Fe^{3+}	0.15	0.10	0.20	0.21	0.46	0.45	0.51	0.53	0.50	0.51	0.44	0.45	0.73	0.72	0.89	
	Fe^{2+}	1.51	1.51	1.58	1.60	1.09	1.05	1.02	0.84	0.92	0.64	0.90	0.83	0.68	0.61	0.87	0.74
	Mg	2.31	2.31	2.38	2.41	2.44	2.50	2.32	2.38	2.65	2.71	2.60	2.67	2.64	2.69	2.59	2.64
	Ti Mg	0.08	0.08	0.03		0.22						0.11		0.15			
	Fe^{3+} (oxy)		0.05														0.89
X	Fe^{2+}						0.07		0.21		0.30		0.10		0.08		0.15
	Ca	1.65	1.65	1.89	1.91	1.73	1.77	1.66	1.70	1.64	1.67	1.54	1.50	1.69	1.73	1.65	1.69
	Na	0.35	0.35	0.11	0.09	0.27	0.15	0.34	0.09	0.36	0.03	0.06		0.31		0.35	0.17
A	Ca												0.09				
	Na	0.49	0.50	0.58	0.62	0.69	0.82	0.32	0.63	0.34	0.73	0.50	0.58	0.37	0.49	0.55	0.74
	K	0.25	0.25	0.13	0.13	0.19	0.20	0.22	0.23	0.21	0.21	0.27	0.28	0.19	0.20	0.24	0.25
OH	OH		1.95		1.47		0.78		0.99		0.93		0.87		1.18		1.11
	F						0.16										0.89
	O^{2-}		0.05														
	Na^{A}	0.74	0.75	0.71	0.75	0.88	1.02	0.60	0.86	0.55	0.91	0.77	1.03	0.56	0.69	0.79	0.99
	Al^{Y}	1.88	1.84	1.77	1.84	1.58	2.25	2.05	2.43	2.06	2.30	1.56	2.24	2.03	2.52	2.22	1.42
	Na^{X}	0.35	0.35	0.11	0.09	0.27	0.15	0.34	0.09	0.36	0.03	0.06	0.00	0.31	0.20	0.35	0.17
	Al^{Z}	1.86	1.86	1.88	1.90	2.20	2.06	2.32	2.20	2.25	2.12	2.27	2.13	2.29	2.18	2.24	2.25
		0.42	0.39	0.50	0.60	0.00	1.06	-0.01	1.00	0.60	1.06	-0.01	1.14	0.00	0.83	0.42	0.00

		42		43		45		46		56		58		59		155	
		23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)
Z	Si	5.56	5.74	5.56	5.71	5.68	5.89	5.56	5.77	5.58	5.75	5.56	5.70	5.62	5.81	5.88	6.05
	Al^{IV}	2.44	2.26	2.44	2.29	2.32	2.11	2.44	2.23	2.42	2.25	2.44	2.30	2.38	2.19	2.12	1.95
Y	Al^{VI}	0.22	0.49	0.27	0.48	0.12	0.42		0.34	0.20	0.45	0.18	0.38	0.16	0.43	0.20	0.44
	Ti	0.46	0.66	0.42	0.64	0.28	0.55	0.30	0.42	0.35	0.57	0.21	0.52	0.27	0.54	0.48	0.59
	Fe^{3+}	1.01	1.05	0.92	0.95	1.15	1.20	1.28	1.29	1.08	1.12	1.12	1.14	1.23	1.28	0.67	0.69
	Fe^{2+}	0.01	0.40	0.51	0.39	0.17				0.28	0.10	0.52	0.53			0.70	0.31
	Mg	2.33	2.40	2.47	2.54	2.76	2.83	2.83	2.76	2.69	2.77	2.38	2.44	2.84	2.75	2.98	3.07
	TiMg	0.18		0.20		0.25		0.29		0.20		0.30		0.25			
	Fe^{2+}		0.23		0.13		0.21		0.18		0.19				0.18		0.41
X	Ca	1.67	1.72	1.79	1.84	1.83	1.79	1.82	1.82	1.77	1.81	1.94	1.99	1.81	1.82	1.56	1.59
	Na	0.33	0.04	0.21	0.03	0.17		0.18		0.23		0.06	0.01	0.19		0.44	
A	Ca						0.11		0.07		0.02				0.06		0.02
	Na	0.37	0.68	0.40	0.63	0.41	0.61	0.46	0.66	0.43	0.67	0.57	0.64	0.45	0.66	0.31	0.77
	K	0.25	0.25	0.22	0.23	0.24	0.24	0.26	0.27	0.22	0.23	0.21	0.22	0.19	0.19	0.29	0.30
OH	OH		0.49		0.78		0.33		0.30		0.61		0.84		0.43		0.70
		Na^A	0.62	0.94	0.62	0.82	0.65	1.07	0.72	1.07	0.65	0.93	0.78	0.86	0.63	0.97	0.61	1.12
		Al^Y	2.15	2.86	2.03	2.71	1.84	2.72	1.89	2.86	1.99	2.70	1.71	2.56	1.94	2.79	1.84	2.12
		Na^X	0.33	0.04	0.21	0.03	0.17	0.00	0.18	0.00	0.23	0.00	0.06	0.01	0.19	0.00	0.44	0.00
		Al^Z	2.44	2.26	2.44	2.29	2.32	2.11	2.44	2.23	2.42	2.25	2.44	2.30	2.38	2.19	2.12	1.95
			0.00	1.50	0.00	1.21	0.00	1.68	-0.01	1.70	0.00	1.38	0.00	1.11	0.00	1.56	-0.09	1.29

		192		270		492		786		944		1493		1603		1667	
		23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)
Z	Si	5.77	5.97	5.67	5.76	5.73	5.87	5.67	5.81	5.71	5.73	6.20	6.26	6.12	6.05	5.76	5.99
	Al^{IV}	2.23	2.03	2.33	2.24	2.27	2.13	2.33	2.19	2.29	2.27	1.80	1.74	1.88	1.95	2.24	2.01
Y	Al^{VI}	0.23	0.51	0.39	0.52	0.38	0.58		0.22	0.38	0.41	0.38	0.47	0.59	0.50	0.22	0.54
	Ti	0.51	0.68	0.72	0.73	0.32	0.54	0.36	0.67	0.32	0.37	0.32	0.46	0.50	0.49	0.32	0.62
	Fe^{3+}	0.04	0.06	0.42	0.42	1.37	0.31	0.93	0.92	0.14	0.14	0.25	0.26			1.32	1.37
	Fe^{2+}	0.74	0.49	2.49	2.31	0.83	0.76	0.17	0.17	1.43	1.44	0.64	0.65	1.46	1.61	0.86	0.68
	Mg	2.58	2.67	0.99	1.01	1.68	1.72	2.83	2.89	2.11	2.12	3.04	3.07	2.45	2.42	1.73	1.80
	TiMg					0.21		0.26	0.06	0.31	0.27	0.19	0.05			0.28	
	$Fe^{3+}(oxy)$						1.39										
X	Fe^{2+}		0.28		0.21		0.09							0.17			0.21
	Ca	1.56	1.61	1.69	1.71	1.47	1.58	1.83	1.92	2.00	2.00	1.85	1.87	1.70	1.68	1.41	1.46
	Na	0.44	0.11	0.31	0.07	0.53	0.40	0.12	0.08			0.15	0.13	0.13	0.32	0.59	0.32
A	Ca									0.14	0.14						
	Na	0.40	0.76	0.09	0.33	0.13	0.27	0.52	0.58	0.64	0.64	0.59	0.61	0.24	0.05	0.16	0.45
	K	0.32	0.32	0.26	0.26	0.28	0.29	0.27	0.28	0.22	0.22	0.09	0.10	0.19	0.19	0.39	0.41
															0.49		
OH	OH		0.46		1.31		0.91		0.93		1.83		1.52		2.00		0.22
	O^{2-}						1.09										
	Na^{A}	0.71	1.08	0.35	0.60	0.41	0.56	0.80	0.86	1.14	1.15	0.68	0.71	0.43	0.73	0.55	0.86
	Al^{Y}	1.89	2.52	2.26	2.41	2.39	1.97	1.65	2.48	1.15	1.28	1.27	1.64	1.58	1.48	2.17	3.14
	Na^{X}	0.44	0.11	0.31	0.07	0.53	0.40	0.12	0.08	0.00	0.00	0.15	0.13	0.13	0.32	0.59	0.32
	Al^{Z}	2.23	2.03	2.33	2.24	2.27	2.13	2.33	2.19	2.29	2.27	1.80	1.74	1.88	1.95	2.24	2.01
		-0.06	1.47	-0.04	0.70	0.00	-0.01	0.00	1.07	0.00	0.16	-0.01	0.48	0.00	-0.06	-0.08	1.68

		1746		* 2189		* 2197		* 2238		* 2305		* 2316	
		23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)	23(O)	24(O)
Z	Si_{IV}	6.36	6.46	5.72	5.86	5.79	5.89	5.80	5.91	5.91	6.03	5.85	5.89
	Al^{IV}	1.56	1.54	2.28	2.14	2.21	2.11	2.20	2.09	2.09	1.97	2.15	2.11
Y	Al^{VI}			0.11	0.21	0.15	0.29	0.12	0.26	0.39	0.55	0.34	0.39
	Ti	0.50	0.51	0.50	0.73	0.54	0.67	0.41	0.55	0.53	0.54	0.63	0.63
	Fe^{3+}	0.47	0.52	0.45	0.46	0.53	0.54	0.33	0.34	0.33	0.33	0.19	0.20
	Fe^{2+}	2.60	2.51	0.91	0.83	1.02	0.92	1.32	1.25	0.93	0.70	1.36	1.25
	Mg	1.43	1.45	2.60	2.67	2.53	2.58	2.55	2.60	2.82	2.88	2.51	2.52
	TiMg			0.21				0.14					
X	Fe^{2+}	0.21	0.35		0.10		0.12		0.89	0.06	0.31		0.12
	Ca	1.70	1.65	1.94	1.90	1.72	1.75	2.00	1.91	1.54	1.56	1.60	1.62
	Na	0.09		0.06		0.28	0.13			0.41	0.12	0.40	0.27
A	Ca		0.07		0.09				0.13				
	Na	0.32	0.44	0.49	0.58	0.38	0.54	0.76	0.78	0.39	0.69	0.41	0.53
	K	0.17	0.17	0.27	0.28	0.31	0.31	0.17	0.17	0.28	0.29	0.31	0.30
OH	OH		1.23		0.37		1.18		1.18		1.11		1.67
	Na^A	0.51	0.76	0.77	1.03	0.69	0.86	0.93	1.21	0.68	0.98	0.71	0.84
	Al^Y	1.48	1.55	1.57	2.24	1.76	2.16	1.26	1.76	1.77	1.96	1.79	1.85
	Na^X	0.09	0.00	0.06	0.00	0.28	0.13	0.00	0.00	0.41	0.12	0.40	0.27
	Al^Z	1.56	1.54	2.28	2.14	2.21	2.11	2.20	2.09	2.09	1.97	2.15	2.11
		0.35	0.77	0.00	1.13	-0.04	0.78	-0.01	0.82	-0.04	0.85	-0.05	0.32

		2342 (C)	2342 24(C)	2717 23(C)	2717 24(C)	2761 23(C)	2761 24(C)
Z	Si	6.09	6.18	5.39	5.56	5.62	5.80
	Al^{IV}	1.91	1.82	2.61	2.44	2.38	2.20
Y	Al^{VI}	0.11	0.22		0.32		0.34
	Ti	0.59	0.60	0.31	0.67	0.61	0.71
	Fe^{3+}	0.51	0.52	1.40	1.39	0.77	0.71
	Fe^{2+}	3.27	3.12	0.16	0.10	0.86	0.55
	Mg	0.51	0.52	2.45	2.53	2.61	2.69
	Ti Mg			0.34		0.08	
X	Fe^{2+}	0.27	0.48		0.07		0.34
	Ca	1.44	1.46	1.84	1.90	1.67	1.66
	Na	0.29	0.06	0.16	0.04	0.33	
A	Ca						0.07
	Na	0.14	0.36	0.48	0.63	0.33	0.67
	K	0.25	0.25	0.28	0.28	0.31	0.32
OH	OH		1.30		0.33		0.50
	O^{2-}				0.19		
	Na^A	0.39	0.62	0.76	0.91	0.64	1.13
	Al^Y	1.81	1.96	2.02	3.05	1.98	2.47
	Na^X	0.29	0.06	0.16	0.04	0.33	0.00
	Al^Z	1.91	1.82	2.61	2.44	2.38	2.20
		0.00	0.71	0.00	1.49	-0.08	1.40

Inspection of Table 5.5 shows that while Na^A, Na^X, and Al^Z are quite restricted and range between 0.56 - 1.21, 0.0 - 0.4, and 1.54 - 2.44 respectively Al^Y is more highly variable and ranges between 1.28 - 3.14. The variation in Al^Y coupled with the variation in the hydroxyl content and the iron oxidation ratio shown by the analyses in Table 5.5 suggested that the method used in MINDATA5 to balance oxyamphibole substitution may be in error. Phillips (1963, p. 708) proposed that in oxyamphiboles enough ferric iron must be available to balance the substitution of O^{2-} for OH^- ($Fe^{2+} + OH^- = Fe^{3+} + O^{2-}$) and that no other ion was involved. Subsequently Leake (1968) and Saxena & Ekström (1970) found no simple relation between the total Fe^{3+} content and O^{2-} substitution in the hydroxyl group in calciferous and subcalciferous amphiboles, but such evidence does not exclude the possibility of the substitution envisaged by Phillips. Phillips included the logic of his statement in MINDATA3 by depleting Al^Y by the amount of ferric iron involved and increasing Mg by an

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Schenk (1950); 367, 368, Carmichael (1967a); 371, Carmichael (1967b); 492, Edwards (1938); 650, Fabries (1963); 786, Kaiser; 797, 798, Harrington (1903); 842, Schalder (1914); 850, 851, 855, Hermes (1970); 944, Howie (1963); 1040, Kempe (1968); 1342, Laughlin *et al.* (1971); 1439, 1442, 1444, Mason (1968a); 1454, Mauritz (1911); 1493, Mottana & Edgar (1969); 1565, 1566, Naidu (1954); 1603, Novotny (1949); 1667, 1668, Parsons (1930); 1746, Perchuk *et al.* (1967); 1828, Ridley (1971); 1982 - 1986, 1988, 1989, Schneider (1891); 2131, Streckeisen (1954); 2189, Tomita (1962); 2197, Uchimuzu (1966); 2200, 2201, Valiquette & Archambault (1970); 2238, Vincent (1953); 2252, Washington & Wright (1908); 2305, White *et al.* (1972); 2316, Wilkinson (1961); 2342, Wolff (1929); 2399, 2400, 2403, 2404, Conquere (1971); 2407, 2410, 2412, Frisch (1970); 2662, Holloway & Burnham (1972); 2717, 2718, LeMaitre (1969); 2720, 2721, 2723, 2724, 2726, 2727. Prinz & Nehru (1970); 2761, Wise (1966): * = Data base reference number.

equal amount. In those instances where ferric iron was insufficient to compensate the oxy-substitution an error was raised and the substitution was not made. For want of any evidence to the contrary the same logic was included in MINDATA5, and may account for the high Al^{Y} values of many of the analyses in Table 5.5.

An approximately linear relationship between the iron oxidation ratio and the $OH^- + F^- + Cl^-$ content in the analyses of Table 5.5 is apparent from Fig. 5.9. Amphiboles from plutonic rocks have lower iron oxidation ratios and higher $OH^- + F^- + Cl^-$ than those from phenocryst, xenocrysts and xenoliths associated with extrusive rocks. The one exception, 786 (Kaiser) is from a weathered monchiquite. Closer examination of Table 5.5 reveals that in only three analyses, 34, 41, and 492 is the ferric iron sufficient to compensate the hydroxyl deficiency in this way, and only in these three has the above substitution been made by MINDATA5. Failure to compensate O^{2-} is not because there is insufficient iron present for in none of the analyses is all the iron in the ferric oxidation state. Perhaps this can be explained by a failure to determine fluorine or chlorine but this seems unlikely since in the three instances where fluorine is determined less than 0.2 atoms are present. Saxena & Ekström (1970) found a negative correlation between Ti^{4+} and OH^-. However, no relationship was found between the Ti^{4+} content and O^{2-} substitution in Table 5.5 which would exist if titaniferous amphiboles were capable of crystallising with O^{2-} in place of OH^- balanced by a substitution such as $R^{3+} + OH^- = Ti^{4+} + O^{2-}$, nor does it appear likely that Ti^{3+} was present and later oxidised to Ti^{4+} ($Ti^{3+} + OH^- = Ti^{4+} + O^{2-}$), since the existence of Ti^{3+} in terrestial minerals is doubtful (Dowty & Clark 1973). It is evident from the above that the substitution $Fe^{2+} + OH^- = Fe^{3+} + O^{2-}$) is important in hydroxyl deficient amphiboles and it is suggested that this substitution

Fig. 5.9. Variation of iron oxidation ratio with the sum of $OH^- + F^- + Cl^-$ in amphiboles with titanium in excess of 0.5 atoms.

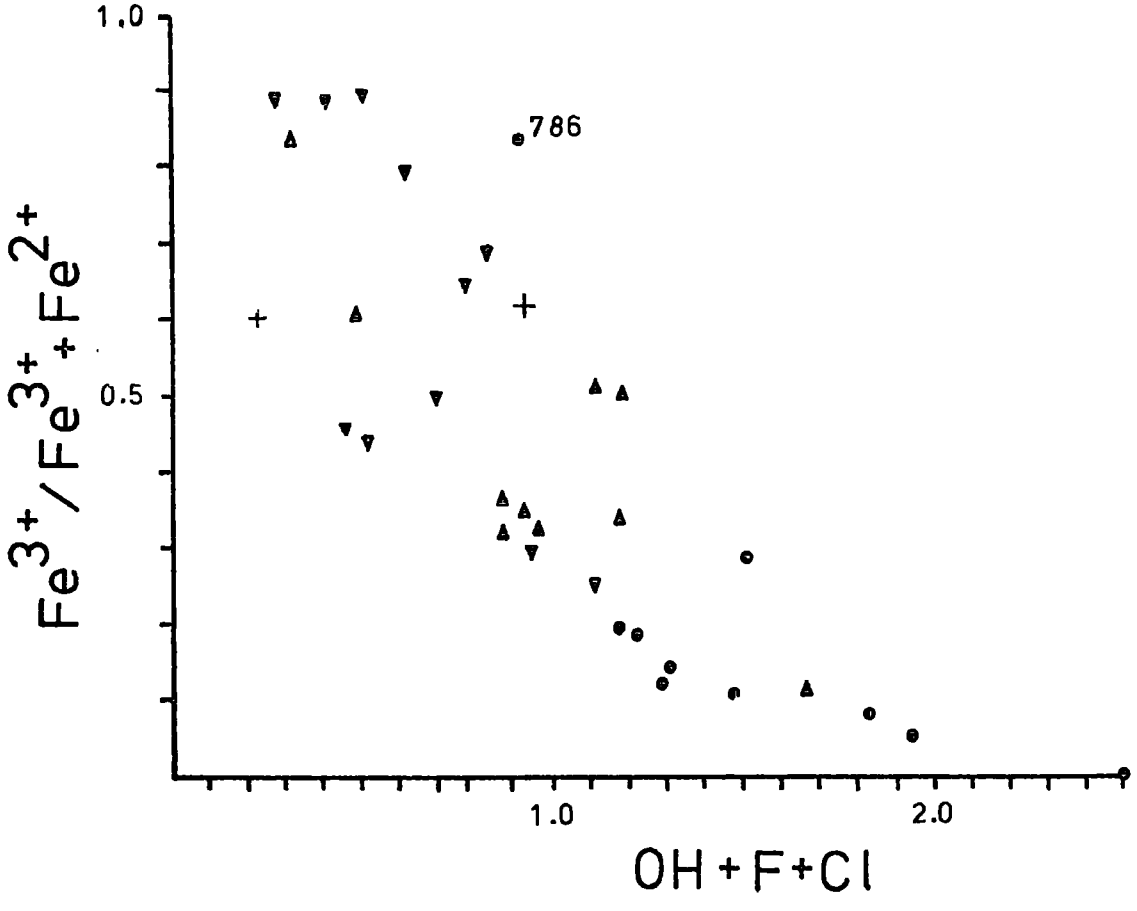
The parageneses of the amphiboles are as follows:-

▲ Phenocrysts in silica undersaturated extrusive rocks

● Silica undersaturated platonic rocks

▼ Xenoliths and xenocrysts including gabbroic, ultrabasic and eclogite bodies.

+ Unknown parageneses.


1.0
0.5
786
1.0
2.0
$Fe^{3+}/Fe^{3+}+Fe^{2+}$
OH+F+Cl

should be made irrespective of whether ferric iron excedes the hydroxyl group deficiency or not. Perhaps the failure of the available ferric iron to excede the hydroxyl deficiency may be attributed to inaccurate water determination and if so emphasises the difficulties involved in using a 24(O) recalculation base and the need for accurate water determinations on amphiboles.

After correcting the Al^Y for ferric iron balancing O^{2-} the range of Al^Y in Table 5.5 is 1.14 - 1.99. With four exceptions all 100 analyses with Ti^{4+} in excess of 0.5 atoms in the amphibole data file have $Al^Z > 1.5$, $Al^Y > 1.0$, $Na^X < 0.5$, $Na^A > 0.5$ and $Ca + Na^X > 1.33$. It is evident that these highly titaniferous amphiboles form a well characterised and discrete group of amphiboles with either Pa, Ts or Su as the dominant component of the basic atomic formula. It is suggested therefore that the term kaersutite has some value in amphibole nomenclature for those amphiboles with $Ti^{4+} \geqslant 0.5$, $Al^Z > 1.5$, $Al^Y > 1.0$, $Na^X < 0.5$, $Mg^X < 0.66$, $Na^A > 0.5$ and either Pa, Ts or Su s.d..

Ferro kaersutite is appropriate for the three analyses 280, 1746, 2342, from syenites and the two from unknown parageneses, 492, 1667, which have $Fe^{2+}/(Fe^{2+} + Mg^{2+}) > 0.5$.

Two of the exceptional analyses mentioned above, 1565, 1566, were considered by Leake (1968) to be inferior and this is certainly true of 1565 which yields a Z group total of 7.11 and an A site of 2.23. 1566 shows a charge in balance of 1.26 and must be considered as inferior also. The remaining two, 367, 368, (Carmichael 1967b), are electron microprobe analyses which resemble richterite apart from their high Ti^{4+} content. Neither analysis gives a balanced basic atomic formula and it was not possible to estimate optimum iron oxidation states for these. Kaersutite is inappropriate for these latter analyses.

5.6. An extended compositional space for the amphiboles.

The basic atomic formula was originally developed for the calciferous and alkali amphiboles but can be extended to include all amphiboles by incorporating all divalent cations in the X group as equivalent Ca and lithium in the X and A groups as equivalent Na^X and Na^A respectively. All amphiboles should fall in amphibole compositional space, Fig. 5.1.

Unfortunately in such a representation the important feature of the occupancy of the X group would not be apparent. Tremolite - ferro tremolite, cummingtonite - grunerite and anthophyllite-ferroanthophyllite would all plot as the same point and the miscibility relations between the calciferous, alkali, cummingtonite and orthorhombic amphiboles would not be indicated. It is generally accepted that the occupancy of the X group determines the symmetry of amphiboles, Thus Ca^{2+}, Na^+ amphiboles including compositions in which the group is occupied jointly by Ca^{2+}, Mg^{2+} ($P2_1/m$ cummingtonite, Papike, Ross & Clark 1969), Ca^{2+}, Li^+ (fluor lithium amphiboles synthesised by Gibbs, Bloss & Shell 1960). Na^+, Mg^{2+} (fluor magnesiorichterite, Gibbs, Miller & Shell 1962) are monoclinic. Amphiboles with Li^+ (holmquisite, Whittaker 1969), Mg^{2+} (anthophyllite, Finger 1970a,b) and Mg^{2+}, Li^+ jointly (protoamphibole, Gibbs 1969) are orthorhombic. Cummingtonite - grunerite and clino-holmquistite (Ginzburg 1965) are monoclinic.

Therefore in deriving an extended form of the basic atomic formula it is apparent that Mg^{2+}, Li^+, Ca^{2+} and Na^+ in the X group should be distinguished. Returning the substitution of Li^+ for Na^+ in the A site as equivalent Na^A an extended basic atomic formula can be written as

$$Na^A_{0-1}\ (Ca\ Na^X\ Mg^X\ Li^X)_2(Mg^Y\ Al^Y)_5(Si\ Al^Z)_8\ O_{22}(OH)_2$$

where Mg^X represents small divalent cations such as Mg^{2+}, Fe^{2+}, Mn^{2+}

Li^X represents lithium in X. Lithium in the A and Y groups is returned as Na^A or balanced by trivalent cations respectively. The meaning of the remaining symbols is the same as in the original definition of the basic atomic formula (see Chapter 3).

Combining Na^X and Li^X to begin with and applying the coupled substitution $Ca = Mg^X$ to the nine 'end members' of Phillips & Layton (1964) six additional extreme compositions are possible.

Tr	$\square\ Ca_2Mg_5Si_8O_{22}(OH)_2$	$\square\ Mg_2Mg_5Si_8O_{22}(OH)_2$
Ts	$\square\ Ca_2Mg_3Al_2Si_6Al_2O_{22}(OH)_2$	$\square\ Mg_2Mg_3Al_2Si_6Al_2O_{22}(OH)_2$
R	$Na\ Ca\ Na\ Mg_5Si_8O_{22}(OH)_2$	$Na\ Mg\ Na\ Mg_5Si_8O_{22}(OH)_2$
Ed	$Na\ Ca_2Mg_5Si_7Al\ O_{22}(OH)_2$	$Na\ Mg_2Mg_5Si_7Al\ O_{22}(OH)_2$
Pa	$Na\ Ca_2Mg_4Al\ Si_6Al_2O_{22}(OH)_2$	$Na\ Mg_2Mg_4Al\ Si_6Al_2O_{22}(OH)_2$
Su	$Na\ Ca\ Na\ Mg_3Al_2Si_6Al_2O_{22}(OH)_2$	$Na\ Mg\ Na\ Mg_3Al_2Si_6Al_2O_{22}(OH)_2$

Each obeys amphibole stoichiometry and the first three correspond with previously named amphiboles.

$\square\ Mg_2Mg_5Si_8O_{22}(OH)_2$ anthophyllite (Anth)

In common use for orthorhombic amphiboles approaching this composition. The 'end member' has been synthesised by Greenwood (1963). Cummingtonite may represent the monoclinic analogue, but it is uncertain whether anthophyllite and cummingtonite are strictly isodimorphous. Layton & Phillips (1960) suggested that they are not and that calcium was an essential element in cummingtonite. Schurmann (1968) could not synthesise cummingtonite - grunerite without Ca^{2+} present. More recent experimental studies by Cameron (1971) showed that cummingtonite crystallised with a higher calcium content than anthophyllite from which it was separated by a two amphibole region. No natural or synthetic iron free cummingtonite is known.

$\square Mg_2Mg_3Al_2Si_6Al_2O_{22}(OH)_2$ gedrite (Gd)

In common use for alkali poor, aluminium rich orthorhombic amphiboles near this composition (Ernst 1968). Compositions near gedrite have been synthesised by Hinrichsen (1968).

$NaMgNaMg_5Si_8O_{22}(OH)_2$ magnesio - richterite (Mg-R)

An amphibole near this composition has been synthesised by Iiyama (1963) and Schreyer & Seifert (1968). The monoclinic fluorine analogue has been synthesised by Gibbs, Miller & Shell (1962), and Fedoseev, et al. (1970) and named fluor magnesio - richterite by the former authors.

The remaining three extreme compositions have, as far as the writer is aware, not been named although $NaMg_2Mg_5Si_7Al\ O_{22}(OH)_2$ and $NaMg_2Mg_4Al\ Si_6Al_2O_{22}(OH)_2$ have previously been suggested by Robinson, Ross & Jaffe (1971). A search of the amphibole data file failed to find any basic atomic formulae within $\pm$ 0.5 units of $NaMg_2Mg_5Si_7Al\ O_{22}(OH)_2$ and $NaMgNaMg_3Al_2Si_6Al_2O_{22}(OH)_2$. However three analyses were found within $\pm$ 0.5 units of $NaMg_2Mg_4Al\ Si_6Al_2O_{22}(OH)_2$. The source, paragenesis and atomic formulae for these are shown in Table 5.6. The maximum percentage of the $NaMg_2Mg_4AlSi_6Al_2O_{22}(OH)_2$ component in each of the analyses is only 51, 50 and 58 per cent respectively, although this latter value is reduced to 54 per cent if Ca^{2+} in the A group is neglected. Robinson, Ross & Jaffe (1971) found that natural aluminous orthorhombic amphiboles departed significantly from Gd towards $NaMg_2Mg_4AlSi_6Al_2O_{22}(OH)_2$. Despite the marginal dominance of the component it is suggested that a name should be coined for the extreme composition. Two names are appropriate, (i) soda gedrite, in allusion to the substitution $\square Al^Y = Na^A\ Mg^Y$ from gedrite or (ii) magnesio-pargasite, in allusion to the substitution $Ca = Mg^X$ in pargasite, cf magnesio-richterite. The former name is to be preferred.

Table 5.6. Source and atomic formulae of amphiboles close to

$Na\ Mg_2\ Mg_4\ Al\ Si_6\ Al_2\ O_{22}\ (OH)_2$

*1308, *1309 Lal (1969), from garnet, cordierite, gedrite, biotite and cordierite gedrite biotite metamorphic assembleges, Fishtail Lake, Ontario.

2640 Stout (1972) electron microprobe analysis from a quartz plagioclase, cordierite gedrite biotite garnet chlorite magnetite metamorphic assemblege, Telemark, Norway.

		1308		1309		2640
		23(O)	24(O)	23(O)	24(O)	23(O)
Z	Si	6.16	6.11	6.12	6.09	6.07
	Al^{IV}	1.84	1.89	1.88	1.91	1.93
Y	Al^{VI}	0.64	0.57	0.57	0.52	1.35
	Ti	0.06	0.06	0.09	0.09	
	Fe^{3+}	0.62	0.61	0.72	0.72	
	Fe^{2+}	0.09	0.19	0.34	0.41	1.07
	Mg	3.60	3.57	3.28	3.26	2.58
X	Fe^{2+}	1.87	1.75	1.82	1.73	2.00
	Ca	0.07	0.07	0.09	0.08	
	Na	0.05	0.17	0.10	0.18	
A	Ca					0.03
	Na	0.46	0.34	0.48	0.39	0.52
	K	0.05	0.05	0.02	0.02	
	H^+		0.37		0.21	
OH	OH		2.00		2.00	
	Na^A	0.51	0.76	0.50	0.67	0.56
	Al^Y	1.37	1.30	1.47	1.42	1.35
	Na^X	0.05	0.17	0.10	0.18	0.00
	Al^Z	1.84	1.89	1.88	1.91	1.93
$(Na^A+Al^Y)-(Na^X+Al^Z)$		0.00	0.00	0.00	0.00	-0.01

Combination of Li^X and Na^X in the extended basic atomic formula means that a minimum of four variables (Al^Z, Al^Y, Na^X and Ca^X or Mg^X) are required to represent the analysis uniquely. A number of three dimensional representations involving three of the variables at a time were tried. The most successful, Fig. 5.10, in terms of Na^X, Ca^X and Al^Z plotted along three orthogonal axes, shows the relationship between calciferous, alkali and Mg^X substituted amphiboles. Every point in the space, with the exception of M, is non-unique but corresponds with a range of compositions, each with fixed Na^X, Ca^X and Al^Z but variable Na^A and Al^Y provided charge balance is maintained. Such a diagram is simple to use and useful in illustrating the overall chemical and miscibility relations of the amphiboles as a group, see Chapter 7. Since points within the extended compositional space are not unique, no attempt has been made to subdivide the space into named volumes.

While it is possible to plot all amphiboles in the extended compositional space it is suggested that to avoid overcrowding in and near the plane Tr - Ed - Pa, Ts - Su - M - G, Ec - R that the original amphibole compositional space will be the most appropriate space for illustrating those amphiboles with $Na^X + Ca \geqslant 1.95$ ($Mg^X < 0.05$) and the extended compositional space for those with $Na^X + Ca < 1.95$ ($Mg^X > 0.05$). This arbitary division is used in Chapter 7 when the distribution of natural amphiboles over amphibole compositional space and the extended compositional space is illustrated and discussed.

When lithium substitution in the X group is considered five variables (Al^Z, Al^Y, Mg^X or Ca^X, Na^X, Li^X) are required to represent the analysis. One more is required if lithium in the A site is to be distinguished. Because of the number of variables required no adequate

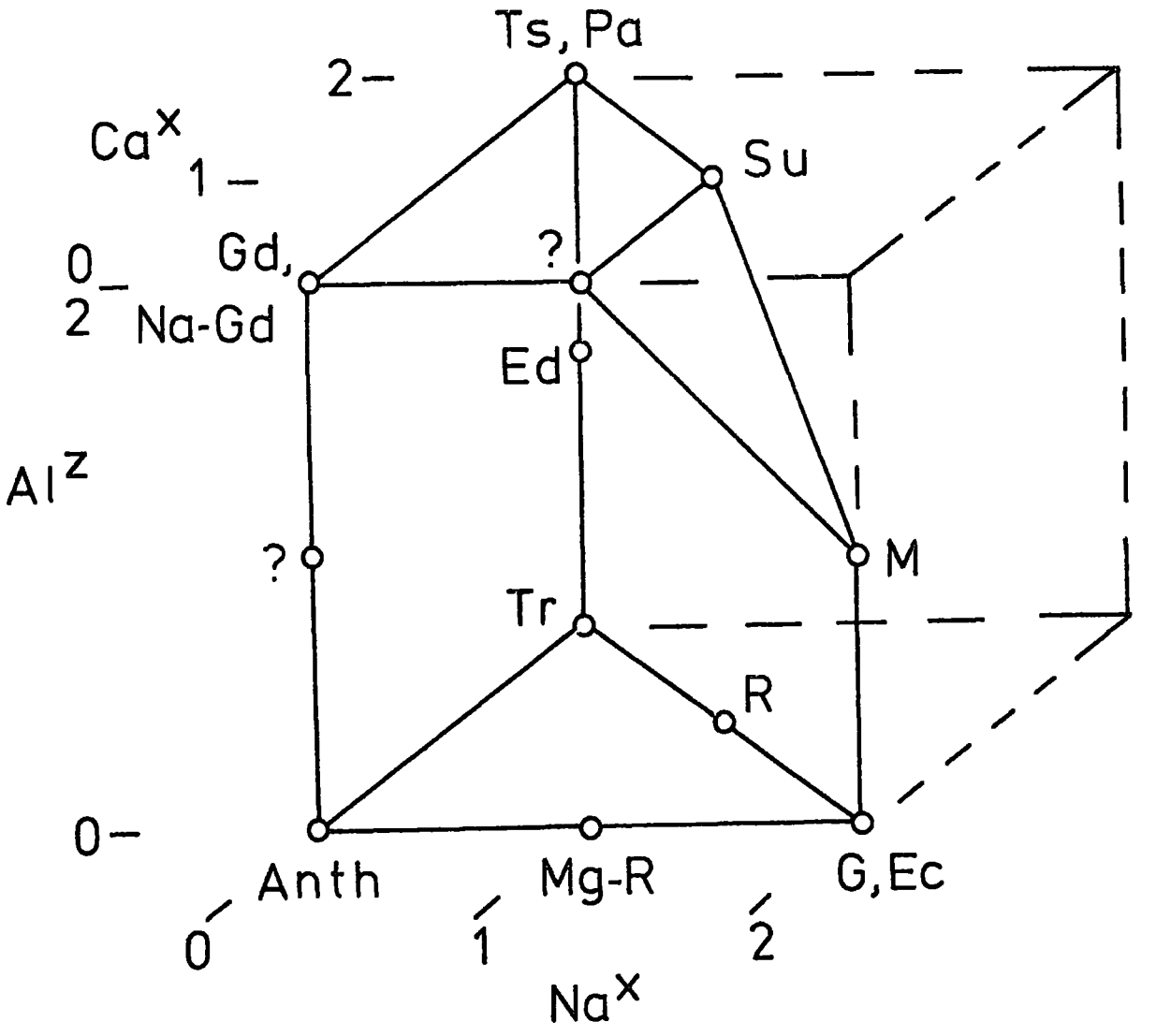


Fig. 5.10. An extended composional space for calciferous, alkali and Mg^X substituted amphiboles.

Abbreviations are the same as Fig. 5.1 with the following additions :- Anth anthophyllite, Gd gedrite, Na-Gd soda gedrite, Mg-R magnesio-richterite, and (?) for the unnamed compositions.

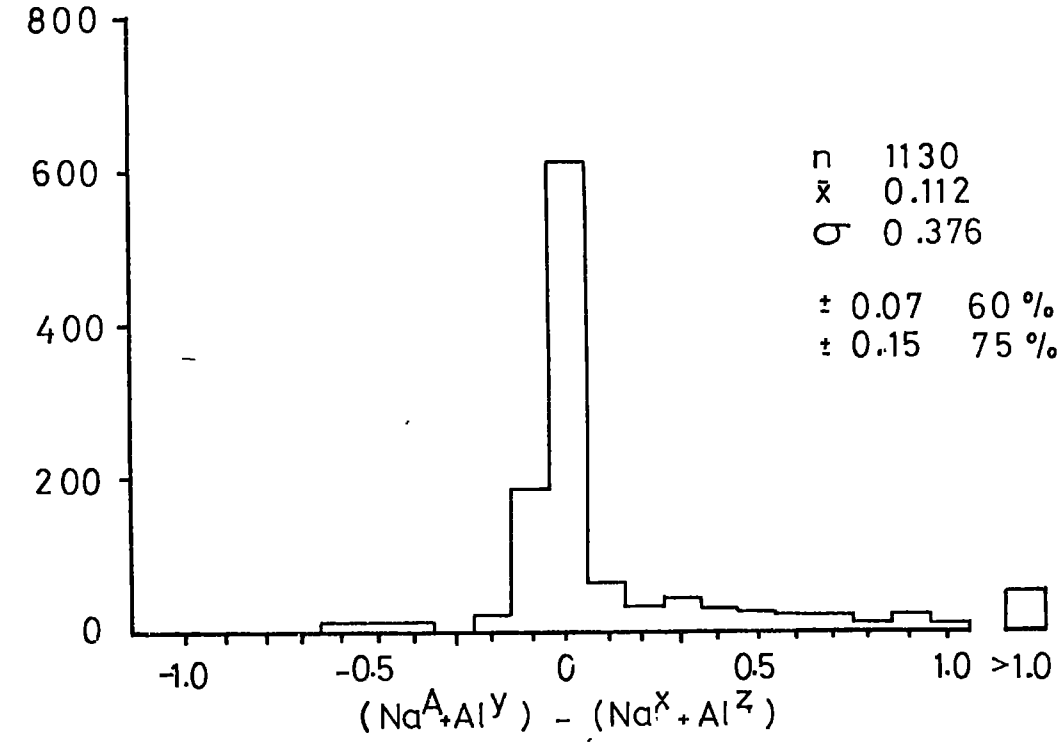
The volume is enclosed within a cube.

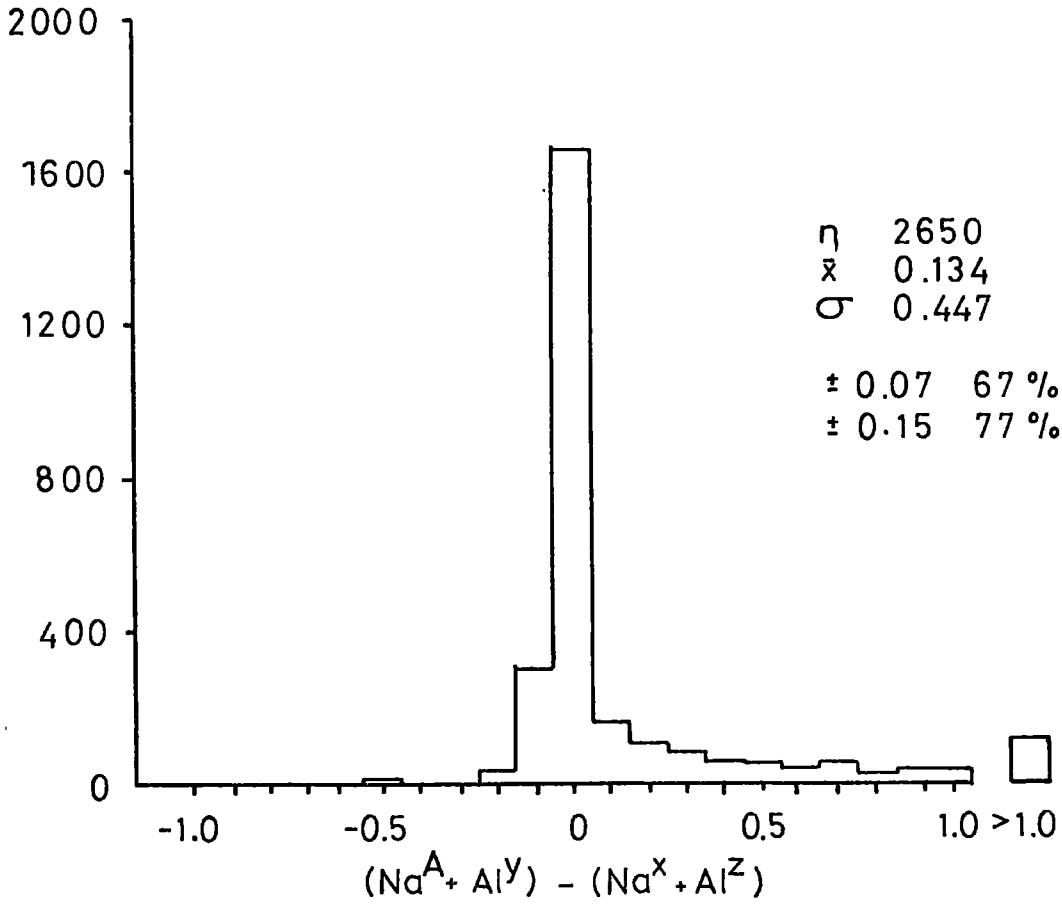
three dimensional representation has been found to show the variation between the calciferous, alkali, Fe^{2+}, Mg^{2+}, Mn^{2+} and Li^{+} substituted amphiboles.

6. BASIC ATOMIC FORMULAE OF ANALYSES IN THE AMPHIBOLE DATA FILE.

Using MINDATA5, (Appendix 4), atomic formulae, basic atomic formulae and values of $(Na^A + Al^Y) - (Na^X + Al^Z)$ were calculated for all 2650 analyses in the amphibole data file, using both 23(O) and 24(O) recalculation bases. When charge balance is achieved the value for $(Na^A + Al^Y) - (Na^X + Al^Z)$ should be zero. In practice (when dealing with real analyses) this is unlikely to be strictly the case and it is therefore necessary to define limits between which analyses may be considered as having achieved charge balance. One approach to this is to assume that the maximum values for Na^A, Na^X, Al^Y, and Al^Z are respectively 1.0, 2.0, 2.0, and 2.0 atoms. A one per cent error in each of the Na^A, Na^X, Al^Y or Al^Z groups will lead to a compounded error in $(Na^A + Al^Y) - (Na^X + Al^Z)$ of $\pm$ 0.07. Using this approach, analyses yielding $(Na^A + Al^Y) - (Na^X + Al^Z)$ outside these limits may be attributed to errors either in the analysis, the allocation scheme, or the method used in deriving the basic atomic formula from the atomic formula. Leake (1965a, 1971) found that errors in amphibole analyses were commonplace. Histograms of the distribution of $(Na^A + Al^Y) - (Na^X + Al^Z)$ calculated to 23(O), for analyses in amphibole compositional space (A.C.S.), defined as $Mg^X <$ 0.05, and for all analyses in both A.C.S. and extended amphibole compositional space (E.A.C.S.) are illustrated in Figs 6.1a and 6.1b respectively. Both distributions are essentially the same and indicate that approximate charge balance is the norm in the amphibole analyses recalculated using MINDATA5. However only 60 and 67 per cent of analyses respectively fall within $\pm$ 0.07. Examination of both distributions suggests that a less rigorous limit of $\pm$ 0.15 might be a more realistic criterion of charge balance as 75 and 77 per cent of analyses fall within this larger limit.

Fig. 6.1. Histograms of $(Na^{A} + Al^{Y}) - (Na^{X} - Al^{Z})$ calculated to 23(O) for (a) amphiboles in amphibole compositional space and (b) amphibole compositional space plus extended amphibole compositional space.


800
600
400
200
0
n 1130
x̄ 0.112
σ 0.376
± 0.07 60 %
± 0.15 75 %
-1.0
-0.5
0
0.5
1.0
>1.0
(Na^A+Al^y) - (Na^x+Al^z)

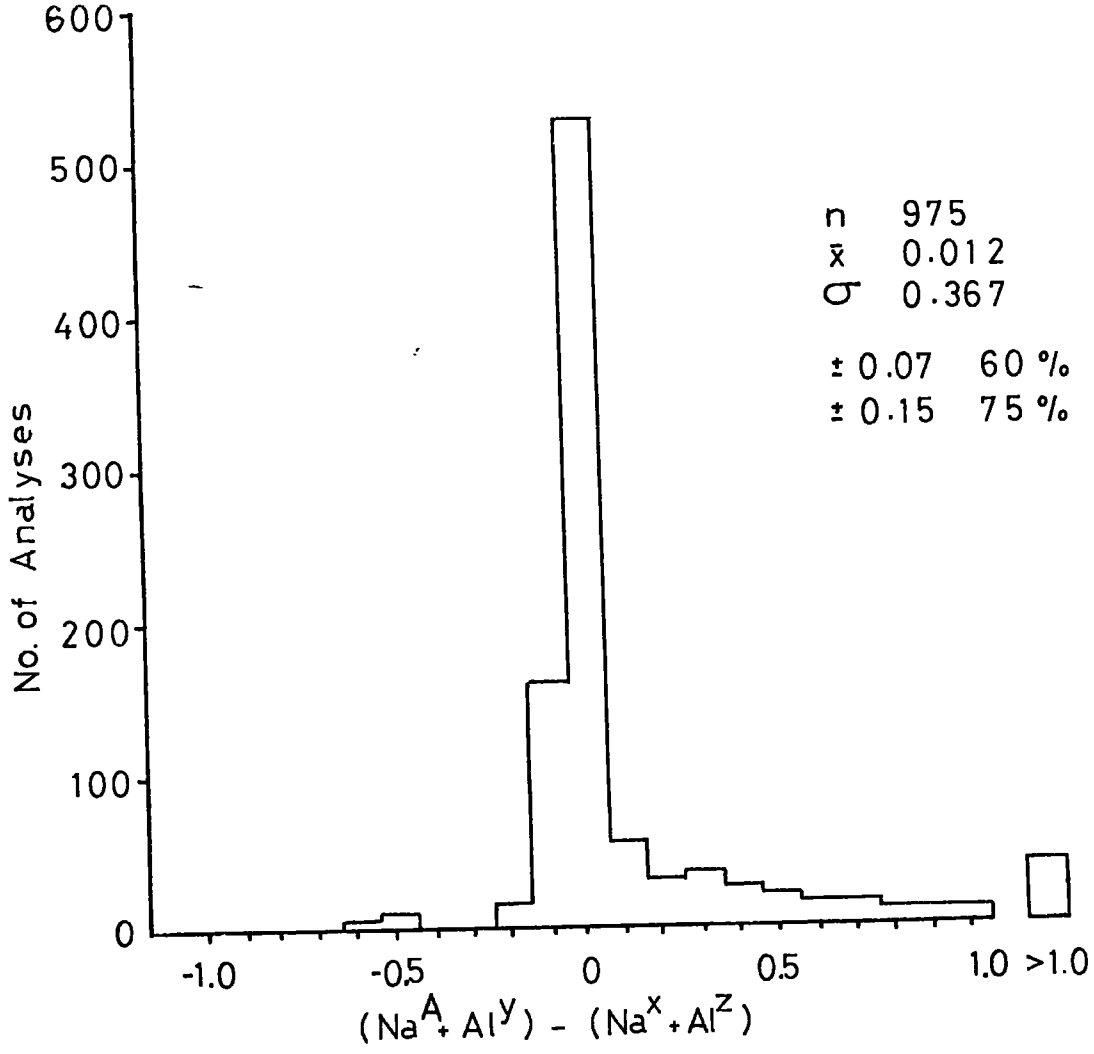

2000
1600
1200
800
400
0
η 2650
x̄ 0.134
σ 0.447
± 0.07 67 %
± 0.15 77 %
-1.0
-0.5
0
0.5
1.0
>1.0
(Na^A+ Al^y) - (Na^x + Al^z)

It is suggested that the positive skewness of the distributions and the unreasonably large deviation from zero for a small number of analyses may be attributed to analytical error. Positive skewness is to be expected as a result of the dependance of the Y on the Z group and the A on the X group in the calculation of the atomic formula, so that errors will tend to accumulate in Na^{A} and Al^{Y}.

A comparison between the charge balance achieved by using a 23(0) and 24(0) recalculation base was undertaken. Figs 6.2a,b give to the base 23(0) and 24(0) respectively, the distribution of $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ for those amphiboles in A.C.S. with either H_2O^{+}, F or Cl determined. Figs 6.3a,b give the same for amphiboles in A.C.S. plus E.A.C.S. The 23(0) distributions, Figs 6.2a, 6.3a are similar to those illustrated in Figs 6.1a,b and show a marked concentration (74 - 75 per cent) of analyses within $\pm$ 0.15. However when recalculated to 24(0) the proportion attaining charge balance is reduced to approximately 50 per cent and in addition in the case of Fig. 6.3b a large number of analyses (in total 380) have $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ in excess of 1.0.

The failure of approximately one half of the amphiboles to attain charge balance when calculated to 24(0) is disquieting. Examination of those analyses with large positive deviations from charge balance (to 24(0)) showed that in many the sum of OH^{-}, F^{-} and Cl^{-} was less than 2.0. In calculating the atomic formula and basic atomic formula using MINDATA5 hydroxyl group deficiency is assumed to be due to the presence of the oxyamphibole substitution of O^{2-} for OH^{-}. From evidence presented in Section 5.5.1 it was suggested that the method used to balance O^{2-} in the hydroxyl group with Fe^{3+}, only when Fe^{3+} exceed O^{2-}, may not be entirely correct. This would tend

Fig. 6.2. Histograms of $(Na^A + Al^Y) - (Na^X + Al^Z)$ for amphiboles in amphibole compositional space with either H_2O+, F^- or Cl^- determined, calculated to (a) 23(O), and (b) 24(O).


600
500
400
300
200
100
0
No. of Analyses
n 975
x̄ 0.012
σ 0.367
± 0.07 60 %
± 0.15 75 %
-1.0
-0.5
0
0.5
1.0
>1.0
(Na^A + Al^y) - (Na^x + Al^z)

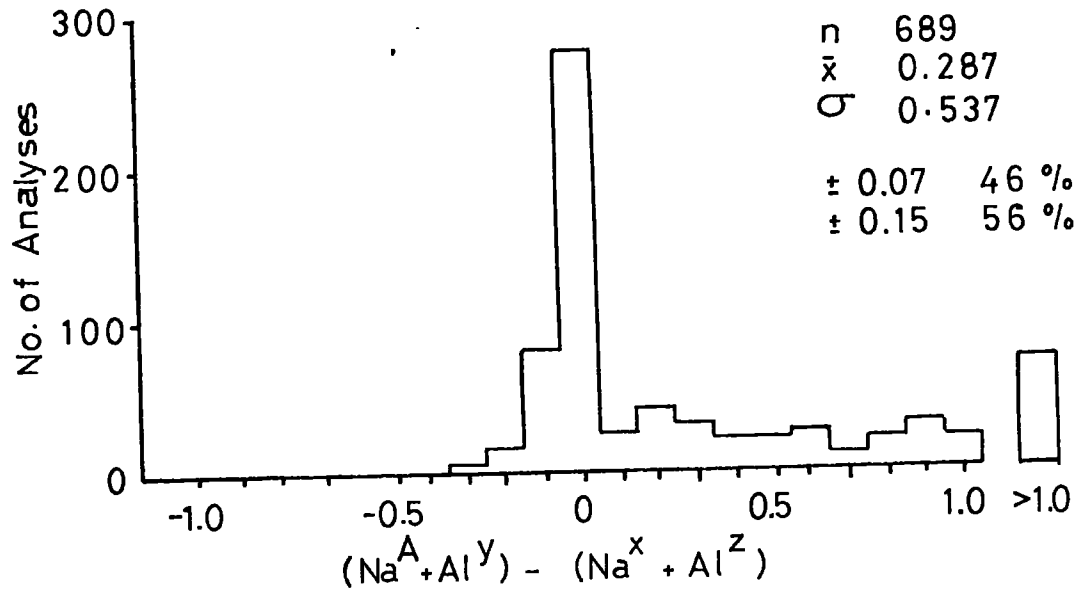
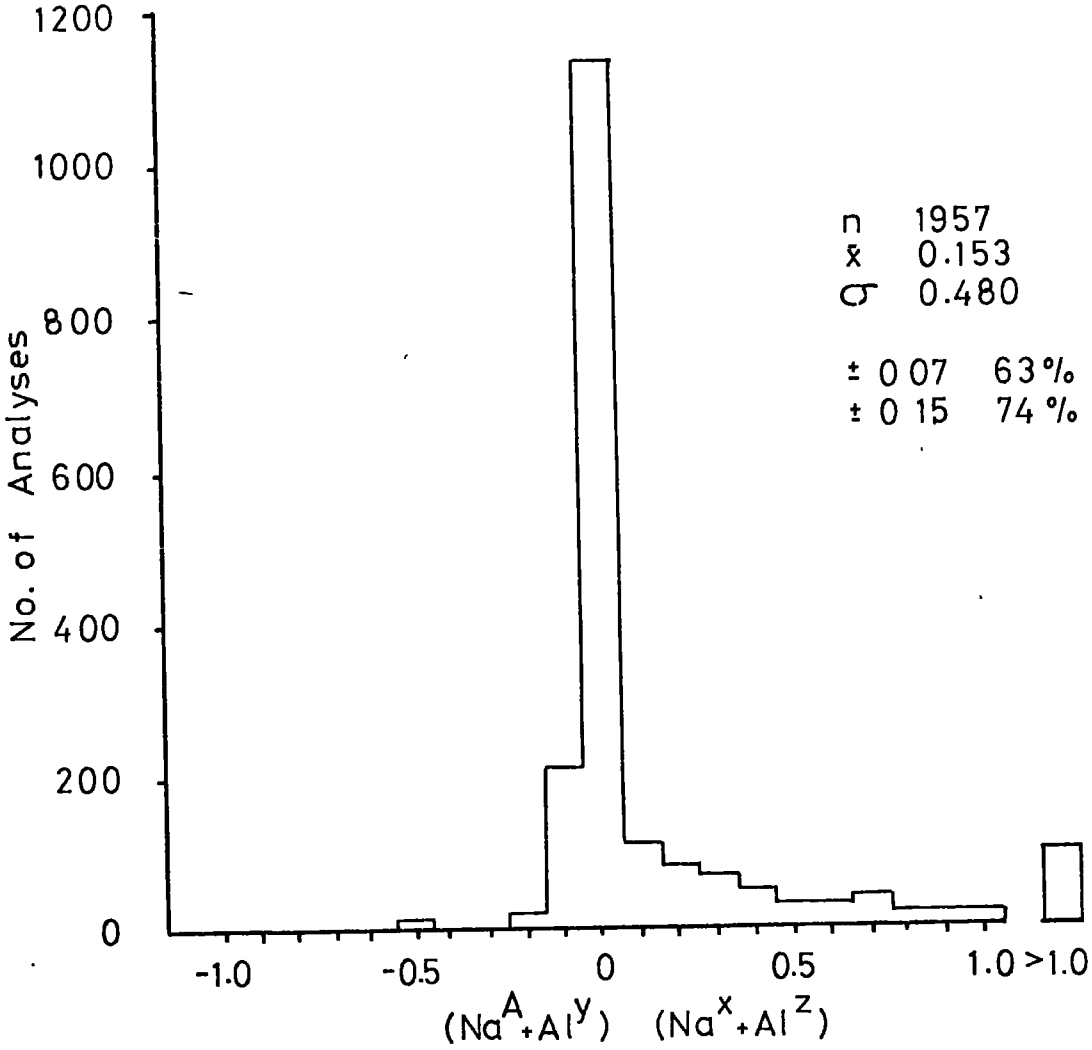
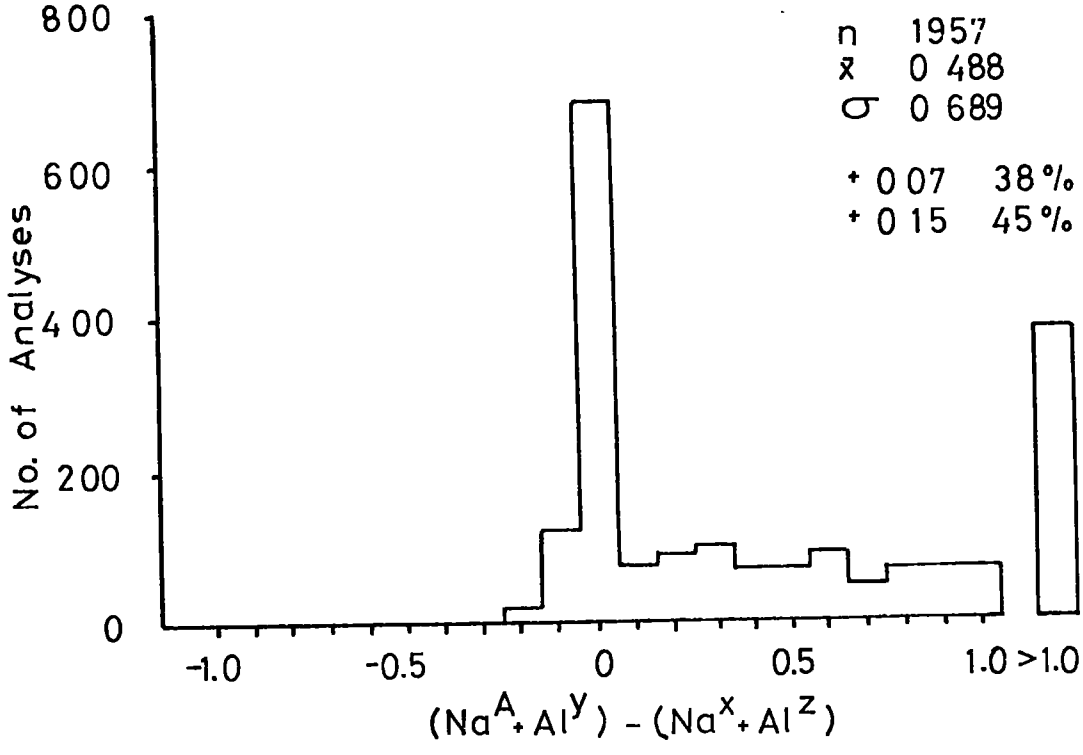

300
200
100
0
No. of Analyses
n 689
x̄ 0.287
σ 0·537
± 0.07 46 %
± 0.15 56 %
-1.0
-0.5
0
0.5
1.0
>1.0
(Na^A + Al^y) - (Na^x + Al^z)

Fig. 6.3. Histograms of $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ for amphiboles in amphibole compositional space plus extended amphibole compositional space with either H_2O+, F or Cl determined, calculated to (a) 23(O) and, (b) 24(O).


1200
1000
800
600
400
200
0
No. of Analyses
n 1957
x̄ 0.153
σ 0.480
± 0 07 63%
± 0 15 74%
-1.0
-0.5
0
0.5
1.0 >1.0
(Na^A + Al^y) (Na^x + Al^z)

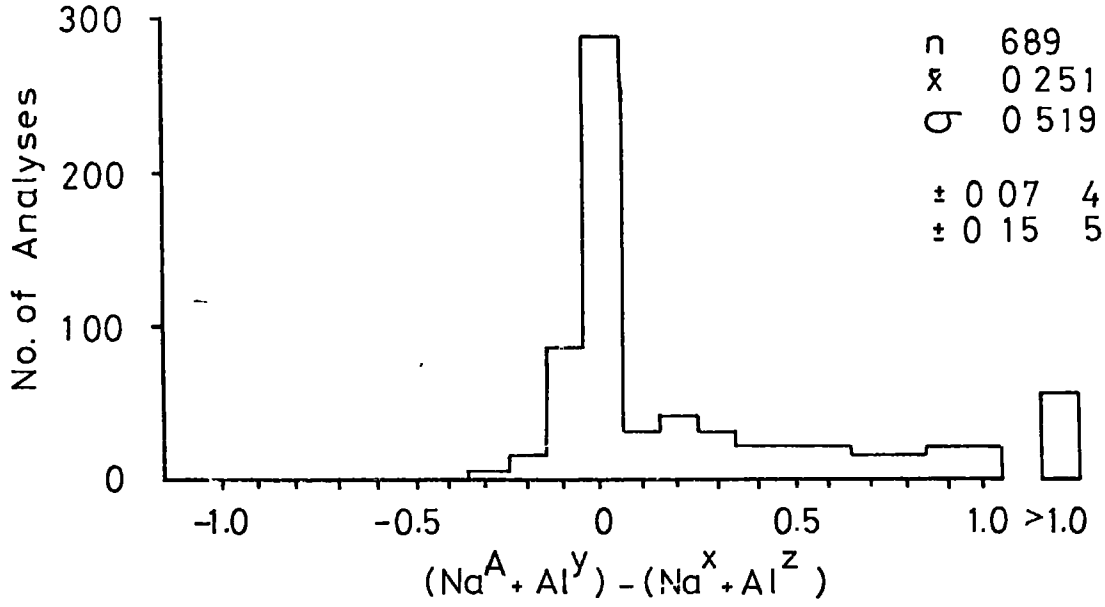

800
600
400
200
0
No. of Analyses
n 1957
x̄ 0 488
σ 0 689
+ 0 07 38%
+ 0 15 45%
-1.0
-0.5
0
0.5
1.0 >1.0
(Na^A + Al^y) - (Na^x + Al^z)

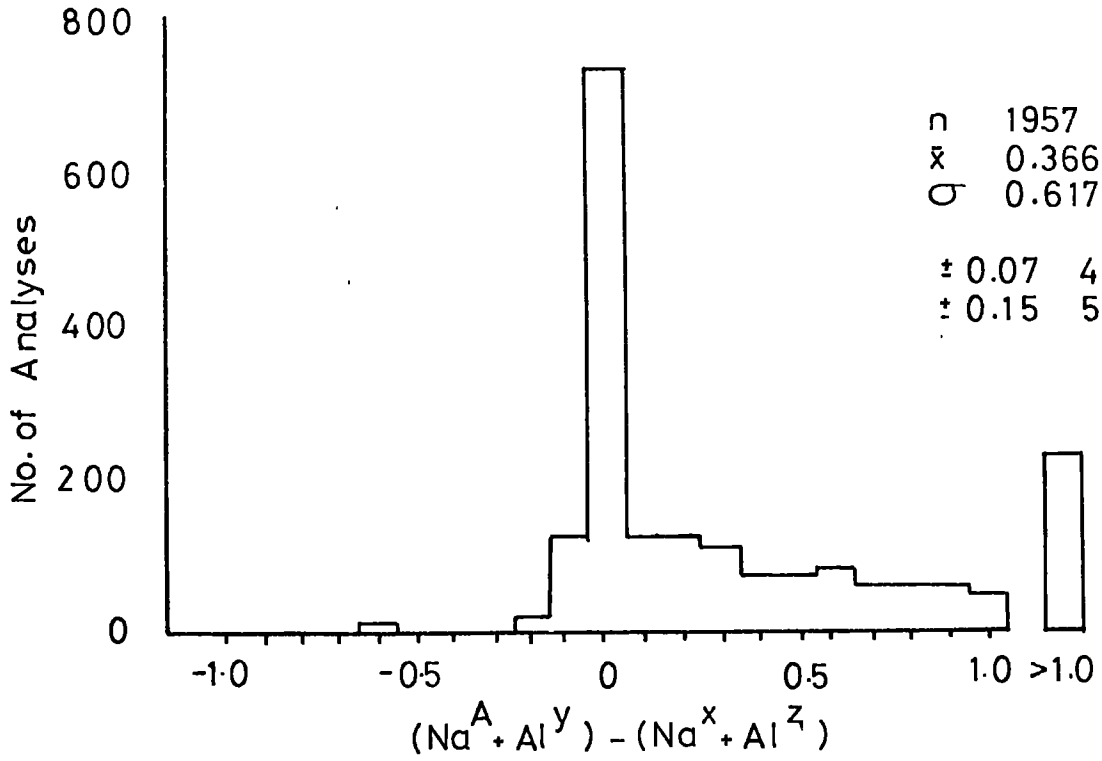
to lead to high Al^Z values and may account for the strong positive skewness observed in Figs 6.2b, 6.3b. By subtracting the Fe^{3+} content from those analyses in which $O^{2-} > Fe^{3+}$ it is possible to determine the effect of this program feature on the distribution of $(Na^A + Al^Y) - (Na^X + Al^Z)$ without reprogramming MINDATA5. The distributions for A.C.S. and A.C.S. plus E.A.C.S. are given in Figs 6.4a,b respectively. A comparison of the proportion of analyses within $\pm$ 0.15 in Figs 6.2a, 6.4a, and 6.3b, 6.4b indicates only a marginal improvement of 2 to 5 per cent and suggests that features other than this idiosyncracy of MINDATA5 must be invoked to explain the failure of many basic atomic formulae to achieve charge balance when calculated to 24(O).

According to Leake (1965a) many water determinations are low because an insufficiently high temperature was not, and is still not, being used to remove all the water in routine analytical techniques and failure to determine fluorine or chlorine will exaggerate this deficiency. Where the hydroxyl site total is inaccurately low the calculated number of cations is high and with the present allocation scheme will tend to accumulate in Na^A and Al^Y. This may account for the positive skewness exhibited in Figs 6.2b, 6.3b, 6.4.

While only Figs 6.3a,b and 6.4b are based on the same analyses and therefore directly comparable it is apparent from the evidence presented above that when considering large numbers of analyses of mixed analytical quality a 23(O) base is more likely to yield balanced basic atomic formulae than a 24(O) recalculation base (see also Robinson Ross & Jaffe 1971). For this reason and the fact that many analyses of amphiboles do not have water, fluorine or chlorine reported a 23(O) recalculation base has been used preferentially throughout the remainder of this work. However, it must be pointed out that a 23(O) recalculation base assumes that

Fig. 6.4. Histograms of $(Na^A + Al^Y) - (Na^X + Al^Z)$ for amphiboles in (a) amphibole compositional space and (b) amphibole compositional space plus extended amphibole compositional space with either H_2O+, F or Cl determined, calculated to 24(O) and assuming that ferric iron always compensates O^{2-} in the hydroxyl group.


300
200
100
0
No. of Analyses
n 689
x̄ 0 251
σ 0 519
± 0 07 48 %
± 0 15 58 %
-1.0
-0.5
0
0.5
1.0
>1.0
(Na^A + Al^y) - (Na^x + Al^z)


800
600
400
200
0
No. of Analyses
n 1957
x̄ 0.366
σ 0.617
± 0.07 42 %
± 0.15 50 %
-1·0
-0·5
0
0·5
1.0
>1.0
(Na^A + Al^y) - (Na^x + Al^z)

OH^- = 2.0 and Borg (1967 a) has shown that the better agreement between the number of atoms in an atomic formula with theoretical limits when calculated to 23(O) may be more apparent than real especially where an error in H_2O^+ is associated with a compensating error in another oxide.

7. THE DISTRIBUTION OF BASIC ATOMIC FORMULAE OF NATURAL AMPHIBOLES IN AMPHIBOLE COMPOSITIONAL SPACE AND EXTENDED AMPHIBOLE COMPOSITIONAL SPACE.

In the present chapter the distribution within amphibole compositional space and extended amphibole compositional space of basic atomic formulae calculated to 23(O) for natural amphiboles with either H_2O+, F or Cl determined is illustrated and discussed (Section 7.1.). The distribution of basic atomic formulae for amphiboles from the major igneous and metamorphic parageneses is also illustrated (Section 7.1), however discussion of this aspect of the amphiboles is deferred until Chapter 8. Using the observed distribution the possibility of a solvus or solvi within amphibole compositional space is considered in Section 7.2.

By including only those analyses with either H_2O+, F or Cl determined the great majority of modern electron microprobe analyses are excluded. Only in special instances where these are of particular interest have optimum iron oxidation states been estimated, since the representation of ranges of basic atomic formulae would have added further confusion to the somewhat overcrowded illustrations which follow.

7.1. The distribution of basic atomic formulae.

In order to indicate the substitution of Fe^{2+} for Mg^{2+} and Fe^{3+} for Al^{vi} in the Y and X groups of atomic formulae, the basic atomic formulae have been subdivided into four categories based on the ratios $Fe^{2+} / (Fe^{2+} + Mg^{2+})$, and $Fe^{3+} / (Fe^{3+} + Al^{vi})$ viz.

$Fe^{2+} / (Fe^{2+} + Mg^{2+})$	$Fe^{3+} / (Fe^{3+} + Al^{vi})$	Abbreviation.
$\leqslant 0.5$	$\leqslant 0.5$	(Mg^{2+}, Al^{vi})
$\leqslant 0.5$	> 0.5	(Mg^{2+}, Fe^{3+})
> 0.5	$\leqslant 0.5$	(Fe^{2+}, Al^{vi})
> 0.5	> 0.5	(Fe^{2+}, Fe^{3+})

To simplify the graphical representation of large numbers of analyses in three dimensional A.C.S. and E.A.C.S. both spaces have been subdivided into slices bounded by upper and lower planes normal to Al^z and each 0.5 units thick. Four slices are required for each space bounded by Al^z 0 - 0.5, 0.5 - 1.0, 1.0 - 1.5, 1.5 - 2.0. An additional slice has been added to both spaces to accommodate analyses with Al^z 2.0 - 2.5. Each slice in A.C.S. is projected onto a two axis plot of Al^y versus Na^x and for E.A.C.S. onto Ca^x versus Na^x. The intersection of the upper and lower faces of each slice with the boundaries of the appropriate space are indicated by full and broken lines respectively. Four plots are given for each slice corresponding to (Mg^{2+}, Al^{vi}), (Mg^{2+}, Fe^{3+}), (Fe^{2+}, Al^{vi}), and (Fe^{2+}, Fe^{3+}) substitution. There are thus 20 two axis plots for A.C.S. and E.A.C.S. The distribution of basic atomic formulae is illustrated in Figs 7.1 - 7.20. It was shown in Chapter 5 that all amphiboles should plot in E.A.C.S. with the amphiboles from A.C.S. in the plane Tr - Ed - Pa, Ts - Su - M - G, Ec - R. To avoid plotting analyses with $Mg^x < 0.05$ twice, amphiboles with $Mg^x < 0.05$ have been plotted in A.C.S. and those with $Mg^x > 0.05$ plotted in E.A.C.S. The zone corresponding to $Mg^x < 0.05$ in E.A.C.S. is vacant therefore.

Other views of A.C.S. and E.A.C.S. are given. Amphiboles with $Na^x \leqslant 0.66$ (the choice of the boundary is discussed below) are projected onto two axis plots of Al^z versus Al^y for A.C.S. (Figs 7.21, 7.22) and Al^z versus Ca^x for E.A.C.S. (Figs 7.23, 7.24). The former resemble the plots of the calciferous amphiboles given by Hallimond (1943), Sundius (1946) and Leake (1962). Basic atomic formulae in A.C.S. are projected onto plots of Al^z versus Na^x (Figs 7.25, 7.26). Lastly those in E.A.C.S. with $Na^x \leqslant 0.66$ and $Mg^x > 1.33$ are plotted as Al^z versus Al^y (Figs 7.27, 7.28).

An attempt has been made to indicate, in a general way, the nature of the host rock from which amphiboles with balanced basic atomic formulae (Chapter 6) were recorded. Amphiboles from igneous rocks are shown by closed symbols and those from metamorphic rocks by open symbols. Further the following more specific categories have been recognised:-

Igneous

- ♦ ultrabasic and ultramafic:- hornblendite, pyroxenite, websterite, agriegite, wherlite, dunite, peridotite, anorthosite etc.
- ■ basic: - tholeiitic basalt, gabbro, norite, dolerite, eucrite, allivalite etc.
  (Where it is not been possible to distinguish between alkali olivine basalt and tholeiitic basalt hosts from the authors' descriptions the amphiboles have been arbitarily included in this category).
- ● intermediate: - andesite, diorite, tonalite, monzonite etc.
- ▼ acid: - rhyolite, dacite, granite, granodiorite etc.
- ◆ basic alkali: - alkali olivine basalt, basanite, tephrite, trachybasalt, trachyandesite, alkali gabbro, teschenite, theralite, lugarite, shonkinite, essexite, urtite, ijolite, camptonite, monchiquite etc.
- ▲ alkali: - trachyte, phonolite, syenite, foyaite, perthosite, pulaskite, mariupolite, carbonatite, fenite etc.

Xenoliths have been included with the appropriate rock type and xenocrysts for want of a better method have been included with the category of the host rock.

Metamorphic

- o general metamorphic assemblages: - typically metabasalts or metapelites from regional and contact metamorphic facies.
- □ eclogites,

Δ calcareous parageneses: - marbles, limestones, dolomites, skarns.

× ferruginious parageneses,

s serpentinites,

+ unknown parageneses.

. unbalanced basic atomic formula with $(Na^{A} + Al^{Y}) - (Na^{X} + Al^{Z})$ > 0.15 (see Chapter 6).

These categories have been chosen in order to distinguish amphiboles from rocks with either markedly differing bulk chemistries or which have been subjected to different physical conditions during crystallisation. The allocation of an amphibole to one of the above categories is based on the name for the host rock used by the original author as included in relation OCCURRENCE, see Chapter 4 and Appendix 9. Consequentialy, it should be emphasised that the allocation is based on the rock type the amphibole was reported to occur in and does not normally take into account whether the phase was primary, secondary, in equilibrium etc. The distribution of basic atomic formulae from the above categories is discussed further in Chapter 8.

Where specific analyses have been mentioned in the text they are accompanied by the data base reference number and the name of the original author. The analysis is also numbered on the appropriate figures and the original data can be located with the aid of Appendix 8.

Considering the large number of points plotted (975 in A.C.S. and 982 in E.A.C.S.), the chemical complexity of the amphiboles, the wide range of host rock chemistry and the range of physical conditions during crystallisation, perhaps the most striking aspect of the distribution is the concentration of basic atomic formulae. Amphiboles are found clustered in three regions with either high Ca^{2+}, (Na^{+}, Li^{+}), or $(Fe^{2+}, Mg^{2+}, Mn^{2+})$ in the X group.

A major compositional break in E.A.C.S. between Mg^{X} 0.4 -

Figs. 7.1 - 7.20. Al^{Y} versus Na^{X} for basic atomic formulae in amphibole compositional space and Ca^{X} versus Na^{X} for basic atomic formulae in in extended amphibole compositional space. Substitution in the atomic formula and Al^{Z} content are as follows:-

7.1	(Mg^{2+}, Al^{vi})	Al^{Z} 0 - 0.5.
7.2	(Mg^{2+}, Fe^{2+})	"
7.3	(Fe^{2+}, Al^{vi})	"
7.4	(Fe^{2+}, Fe^{3+})	"
7.5	(Mg^{2+}, Al^{vi})	Al^{Z} 0.5 - 1.0
7.6	(Mg^{2+}, Fe^{3+})	"
7.7	(Fe^{2+}, Al^{vi})	"
7.8	(Fe^{2+}, Fe^{3+})	"
7.9	(Mg^{2+}, Al^{vi})	Al^{Z} 1.0 - 1.5
7.10	(Mg^{2+}, Fe^{3+})	"
7.11	$(Fe2^{+}, Al^{vi})$	"
7.12	(Fe^{2+}, Fe^{3+})	"
7.13	(Mg^{2+}, Al^{vi})	Al^{Z} 1.5 - 2.0
7.14	(Mg^{2+}, Fe^{3+})	"
7.15	(Fe^{2+}, Al^{vi})	"
7.16	(Fe^{2+}, Fe^{2+})	"
7.17	(Mg^{2+}, Al^{vi})	Al^{Z} 2.0 - 2.5
7.18	(Mg^{2+}, Fe^{2+})	"
7.19	(Fe^{2+}, Al^{vi})	"
7.20	(Fe^{2+}, Fe^{2+})	"

The meanings of the symbols are described in the text. The intersection of the upper and lower faces of each slice with the boundaries of the appropriate space are indicated by full and broken lines respectively.

Fig. 7.1. Al^z 0—0.5. (Mg,Al^{vi})

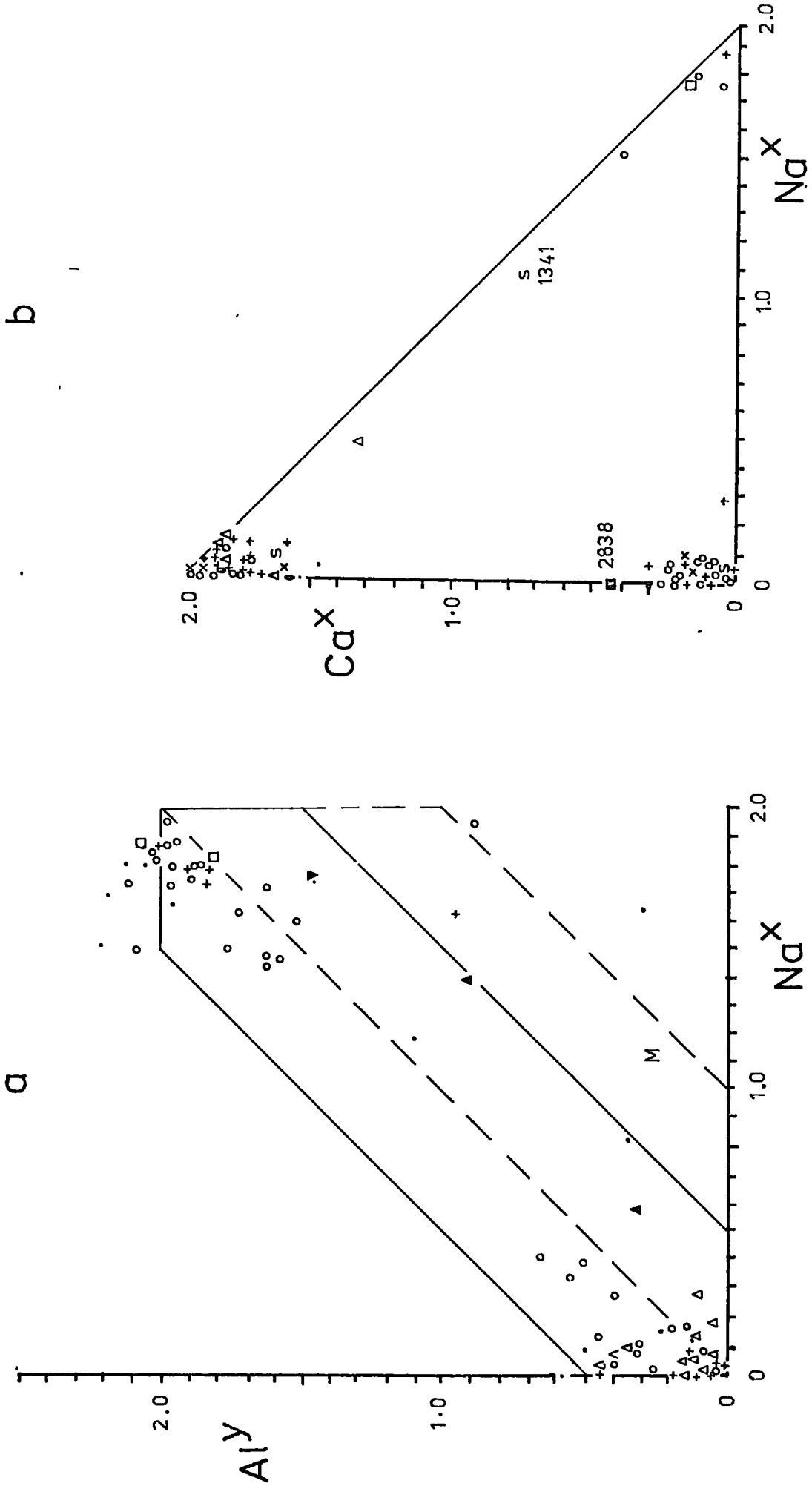
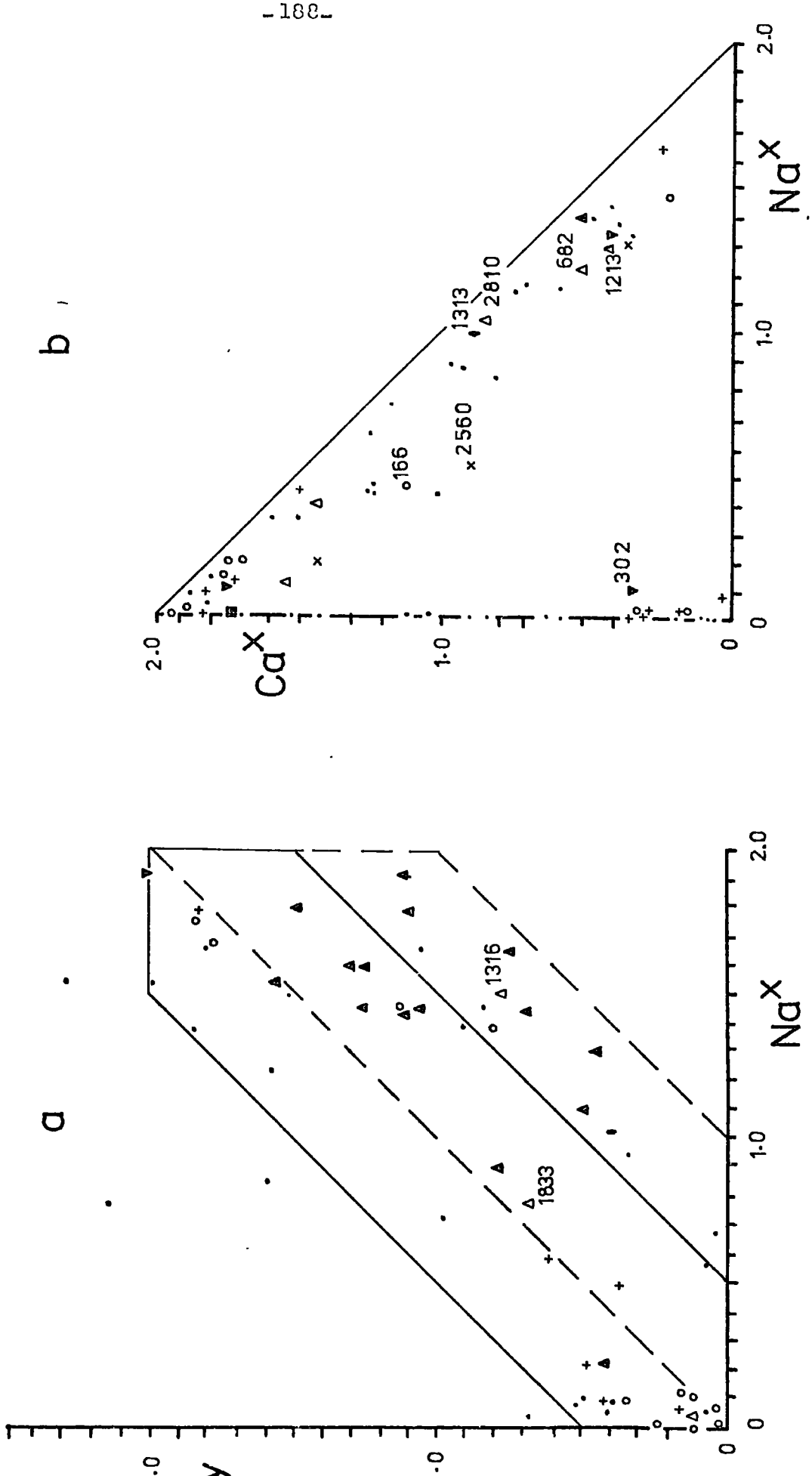


Fig. 7.2. Al^z 0–0 5, (Mg,Fe^{3+})



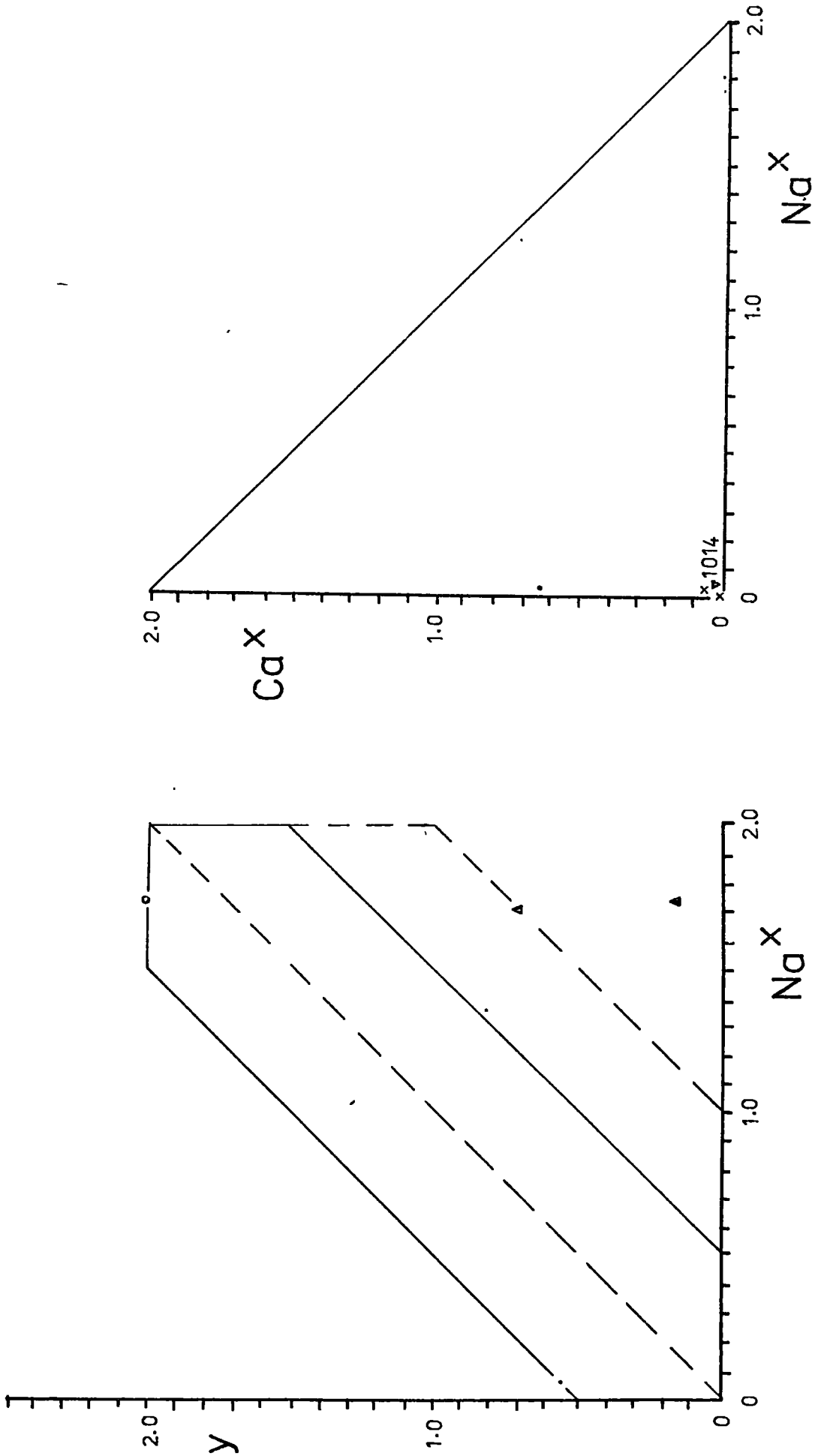

Al^z 0—0 5 . (Fe^2+, Al^vi)
Al^y
Na^x
Ca^x
Na^x
2.0
1.0
0
1×1014

Fig. 7.4. Al^z 0–05. (Fe^{2+},Fe^{3+})

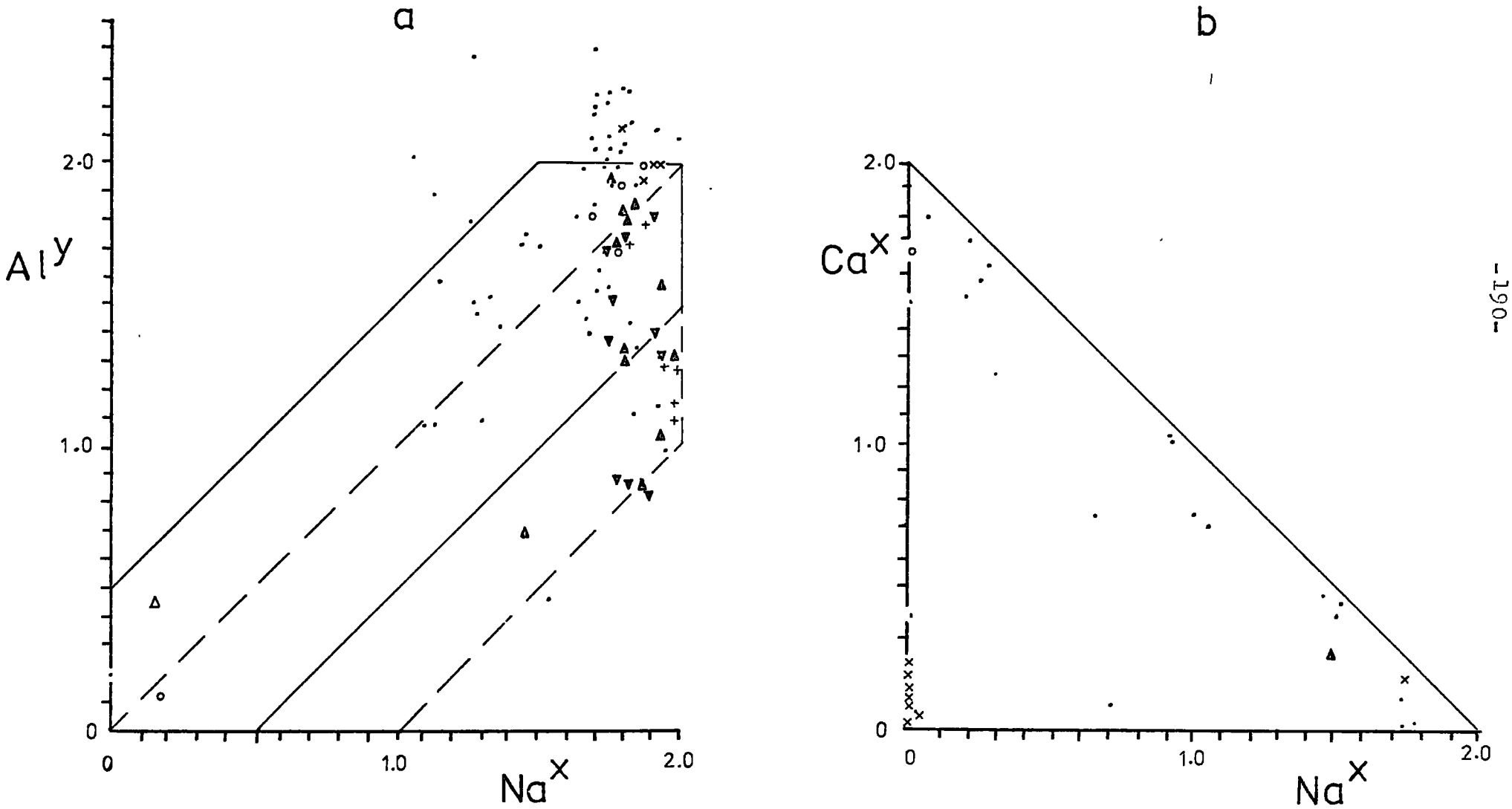


Fig. 7.5. Al^{z} 0.5—1.0, (Mg, Al^{vi})

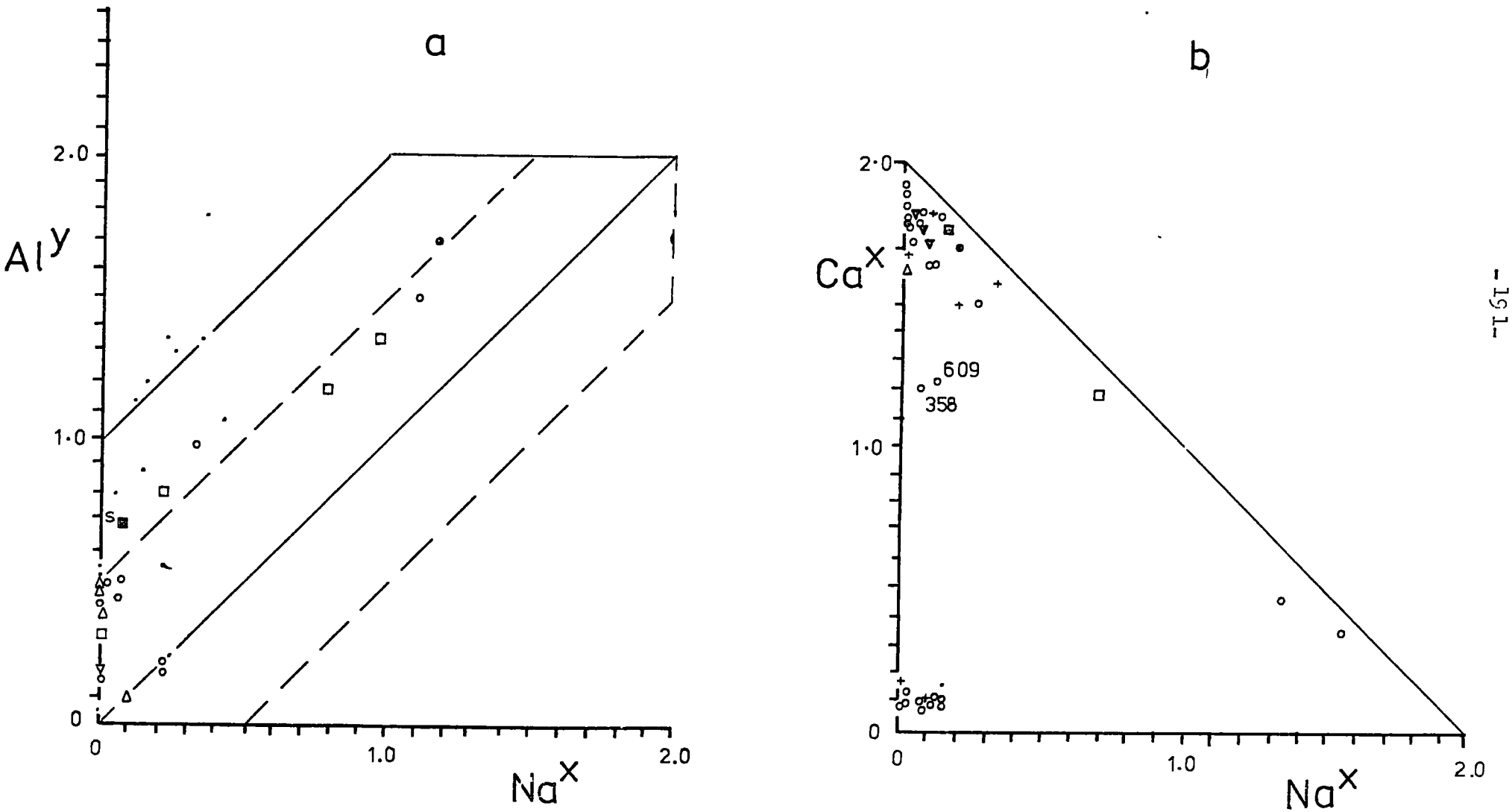
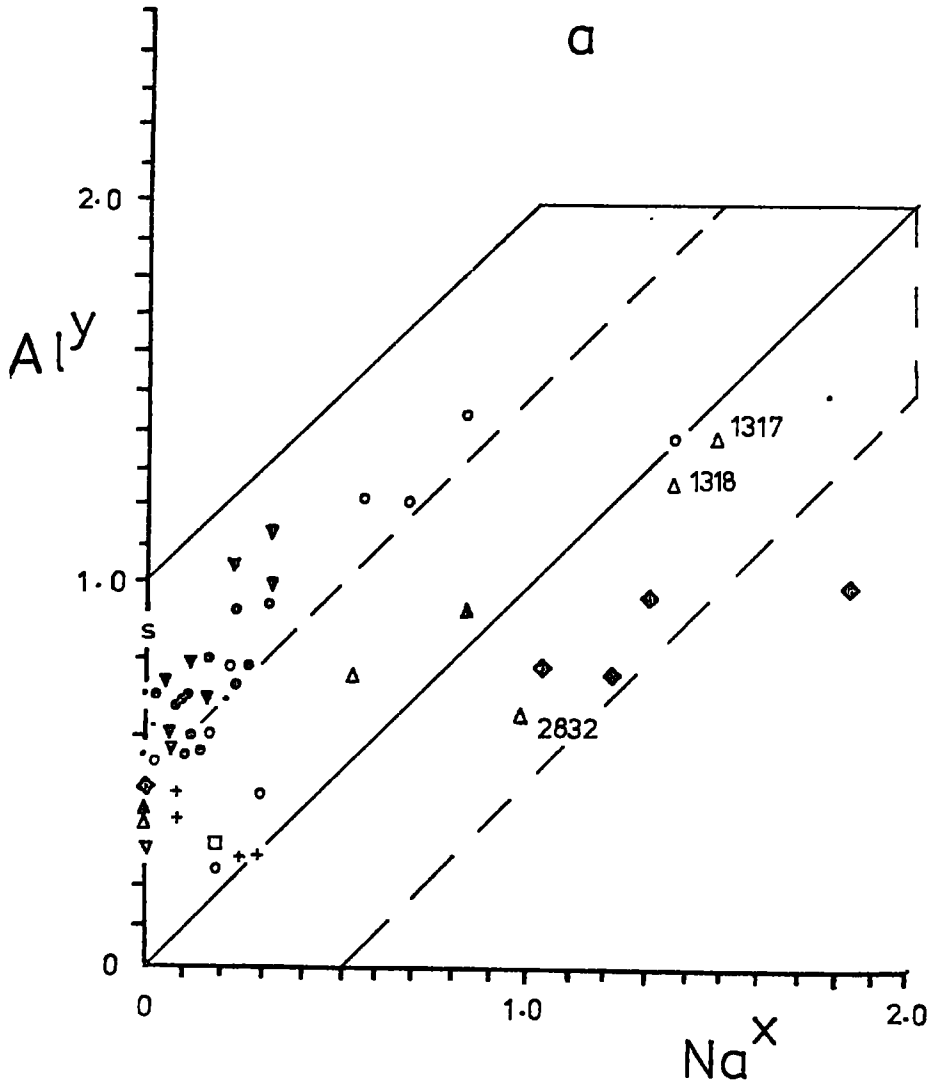


Fig. 7.6. Al^{Z} 0 5—1 0. (Mg,Fe^{3+})



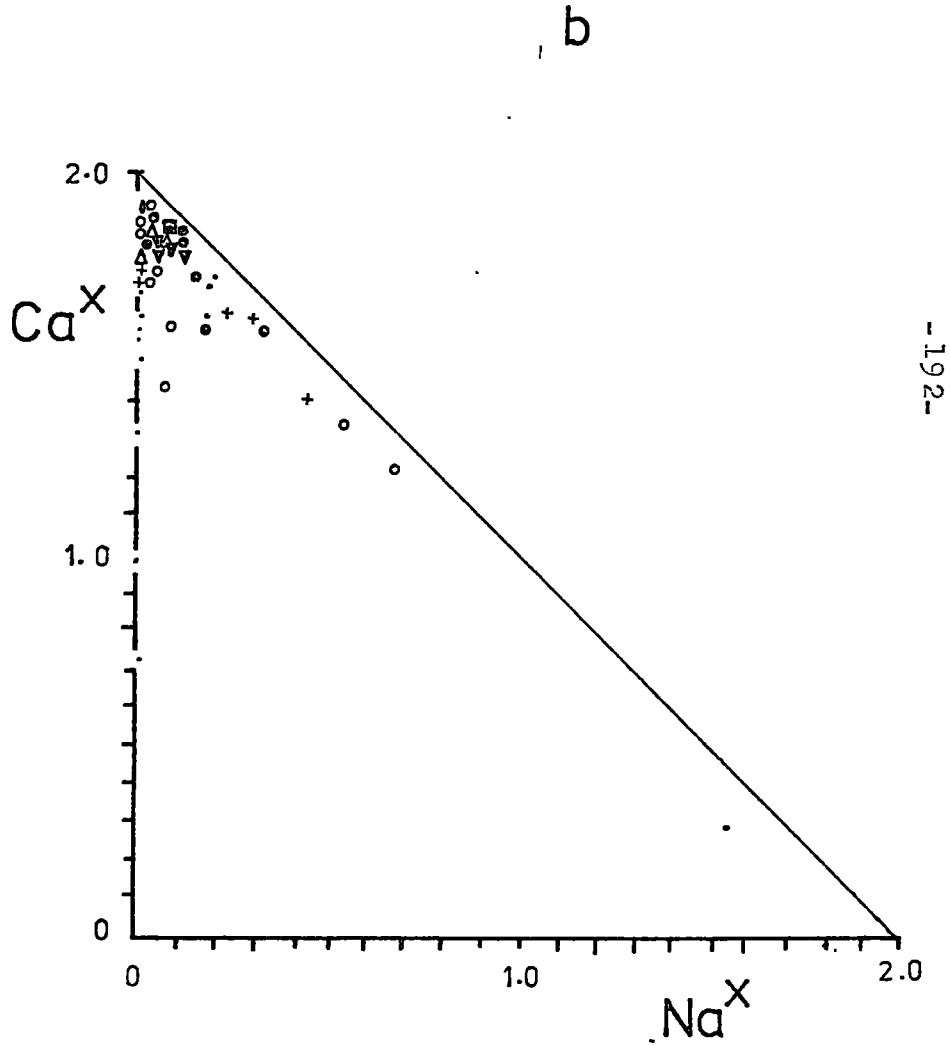


Fig. 7.7. Al^{z} 0.5—1.0 , (Fe^{2+},Al^{vi})

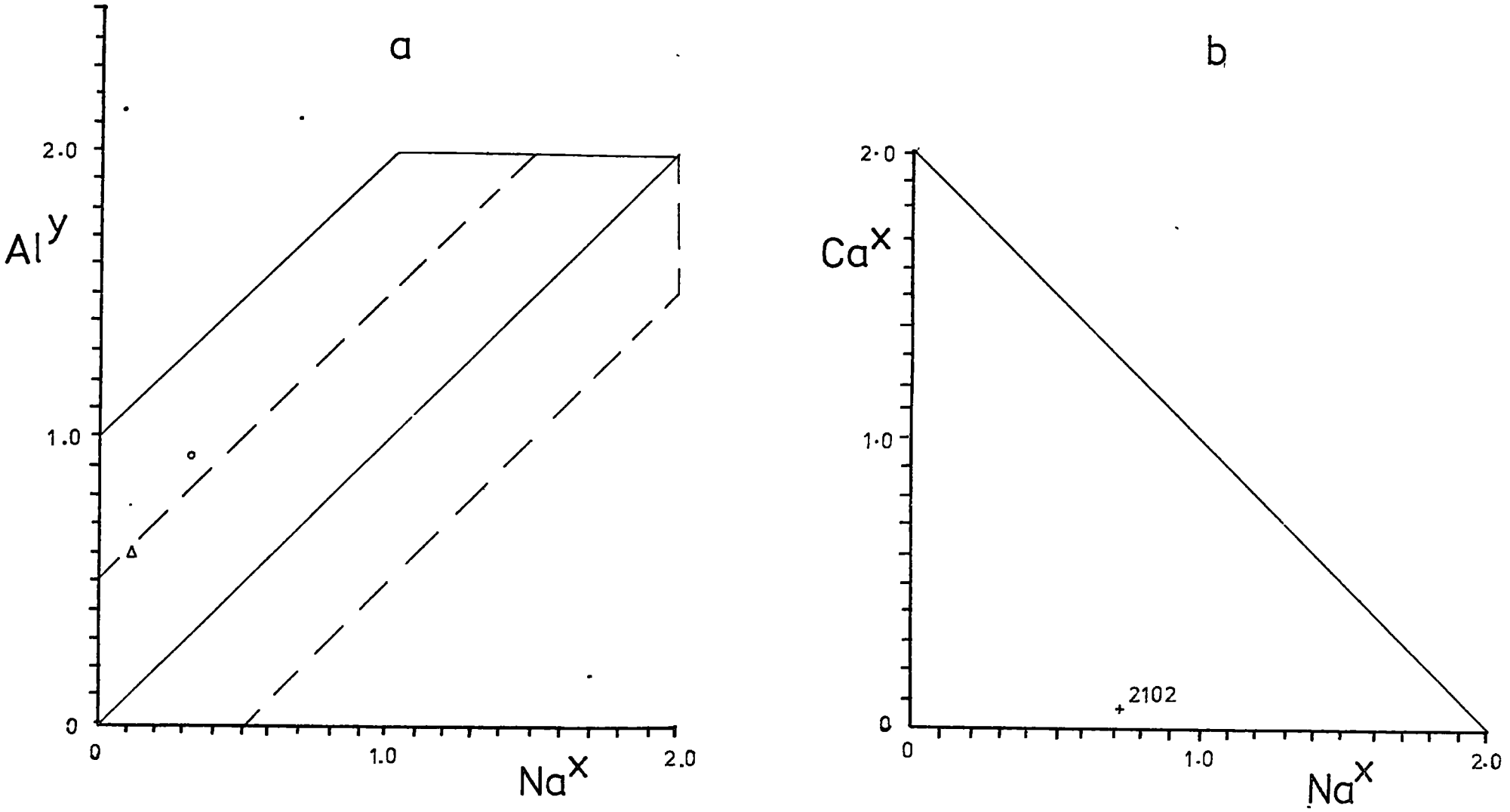
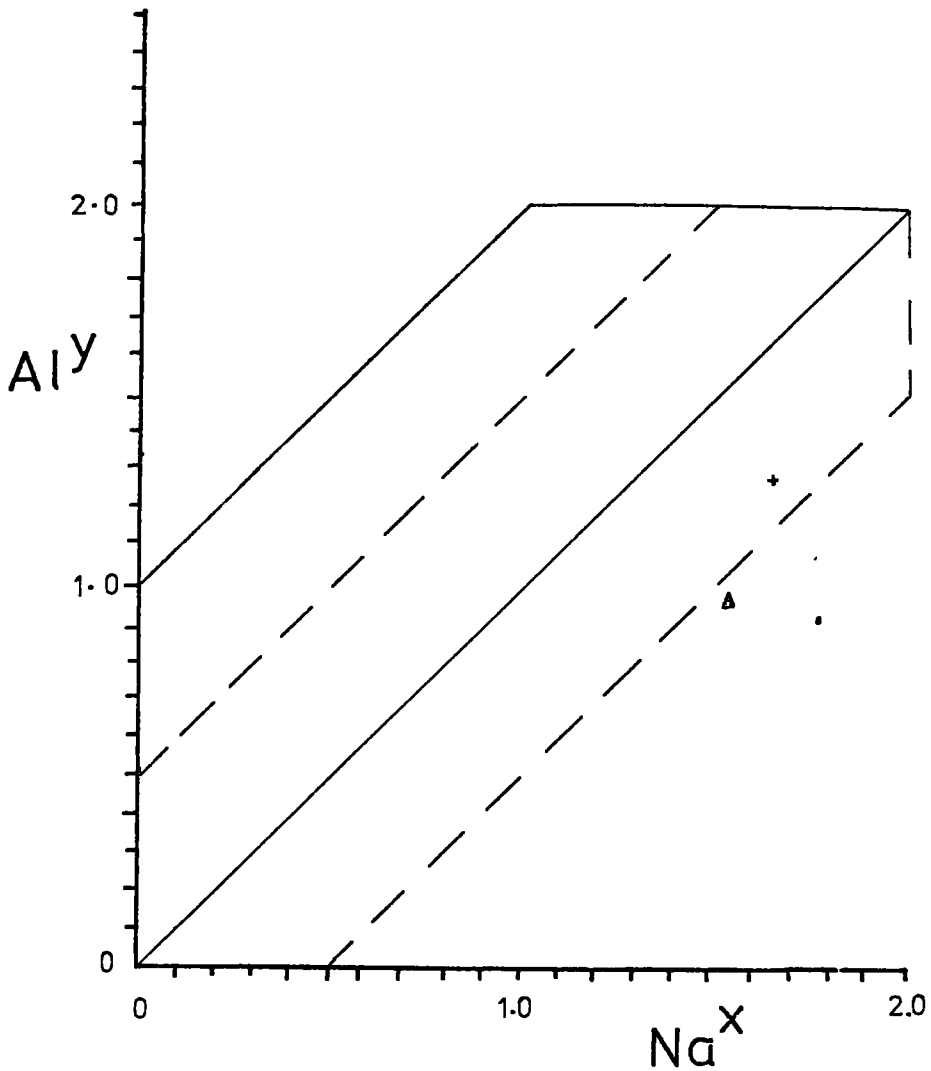


Fig. 7.8. Al^z 0.5—1.0 , (Fe^{2+},Fe^{3+})



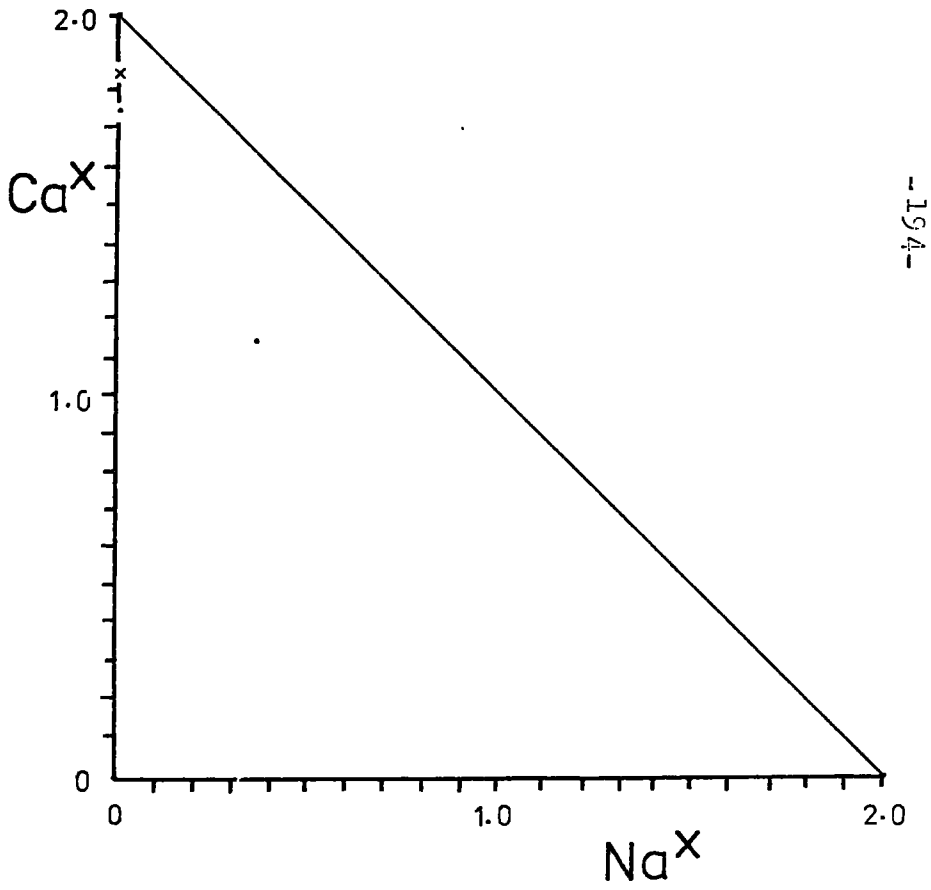


Fig. 7.9. Al^{z} 1.0—1.5 , (Mg,Al^{vi})

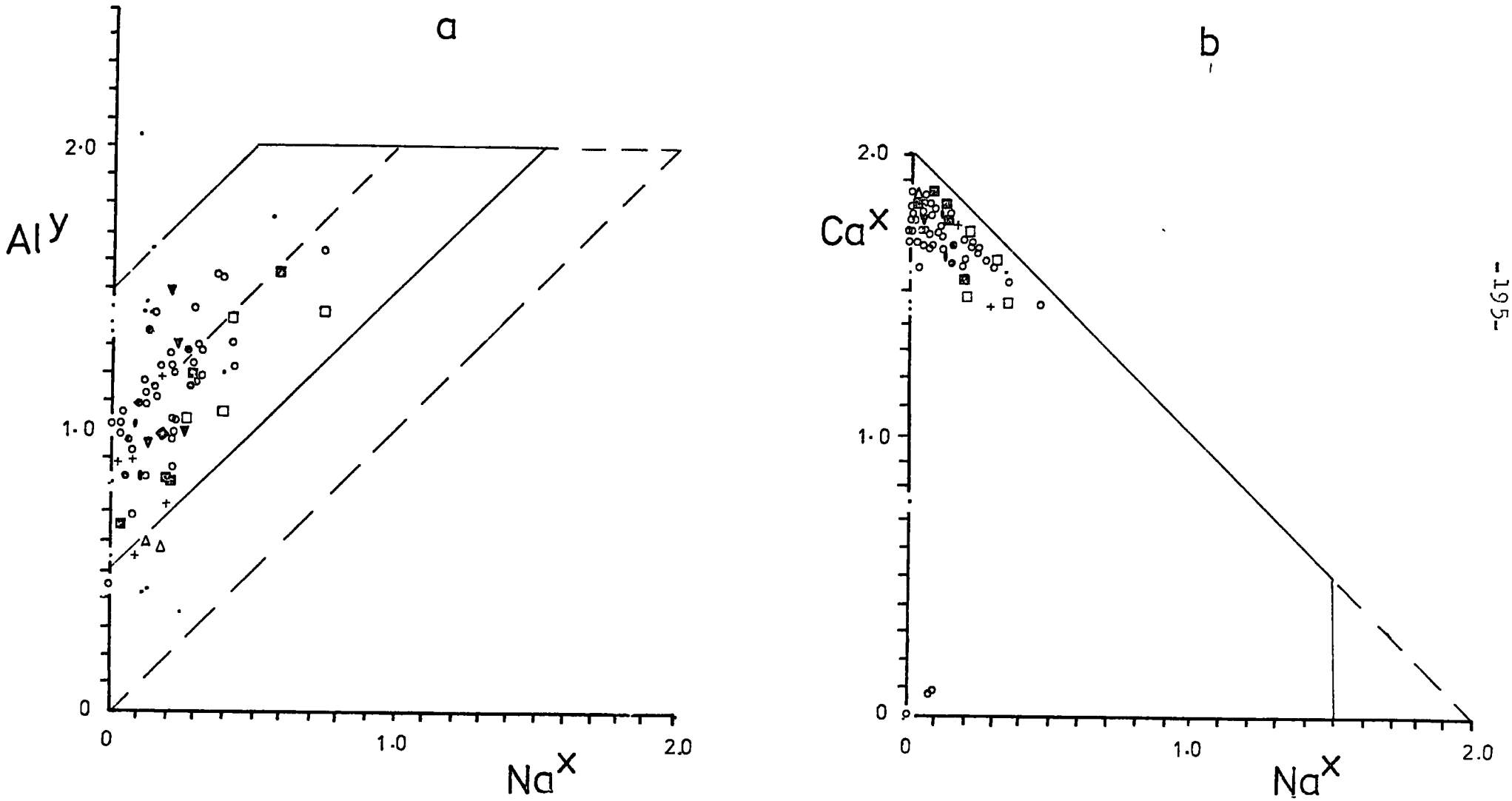
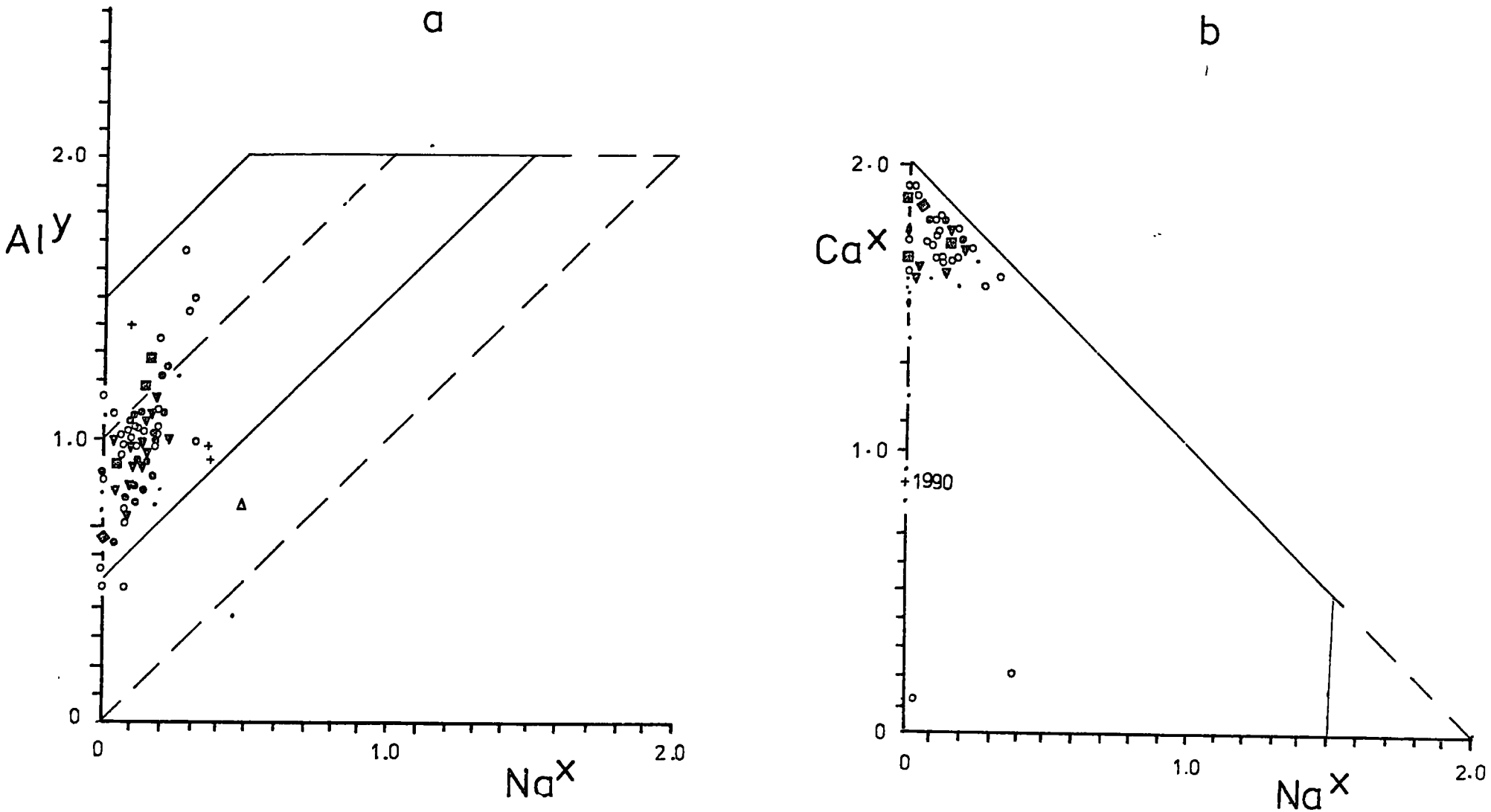


Fig. 7.10. Al^z 1.0—1.5 , (Mg,Fe^{3+})



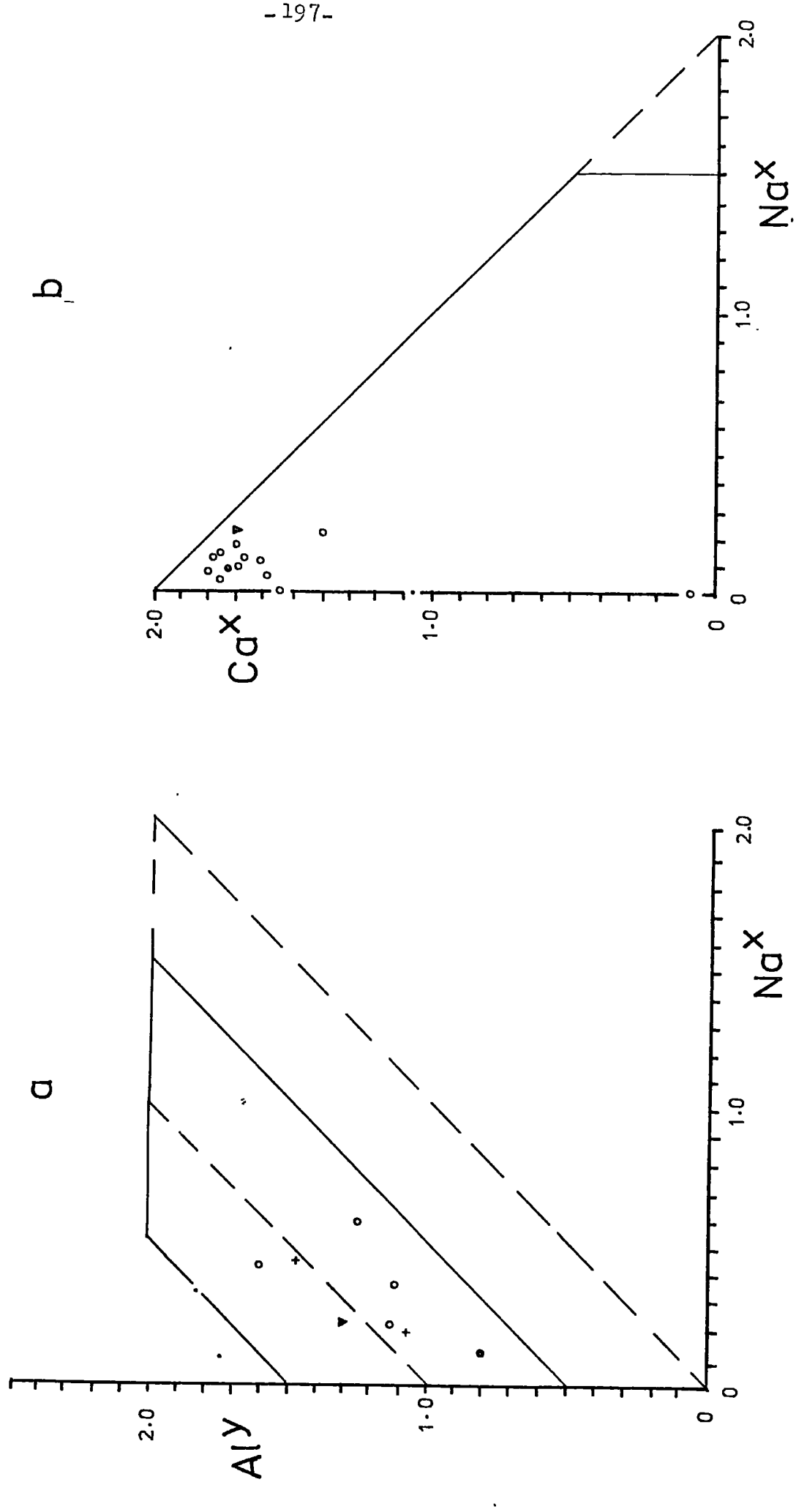
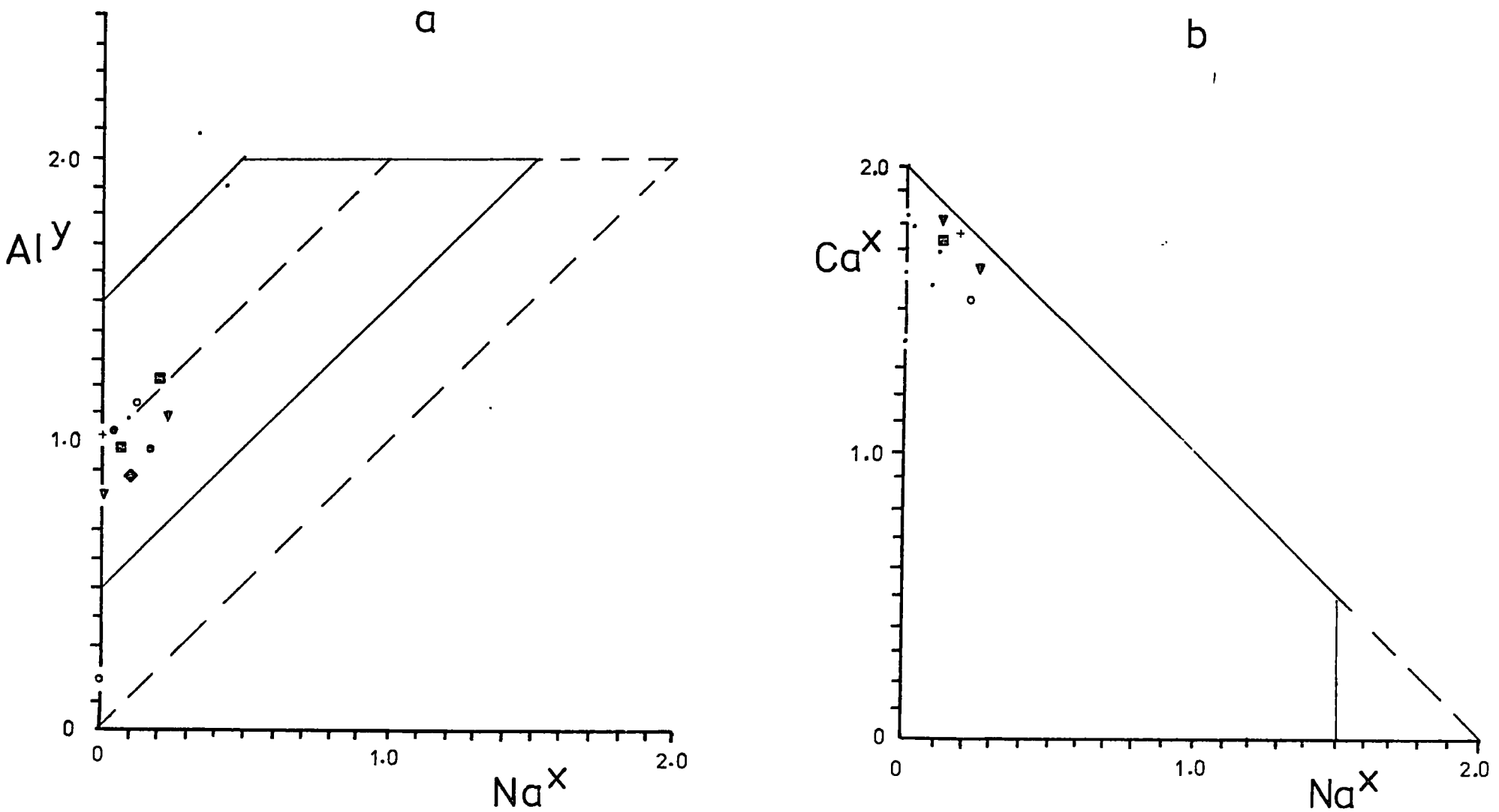


Fig. 7.11. Al^z 1.0—1.5, (Fe^{2+},Al^{vi})

Fig. 7.12. Al^z 1.0—1.5 , (Fe^{2+},Fe^{3+})



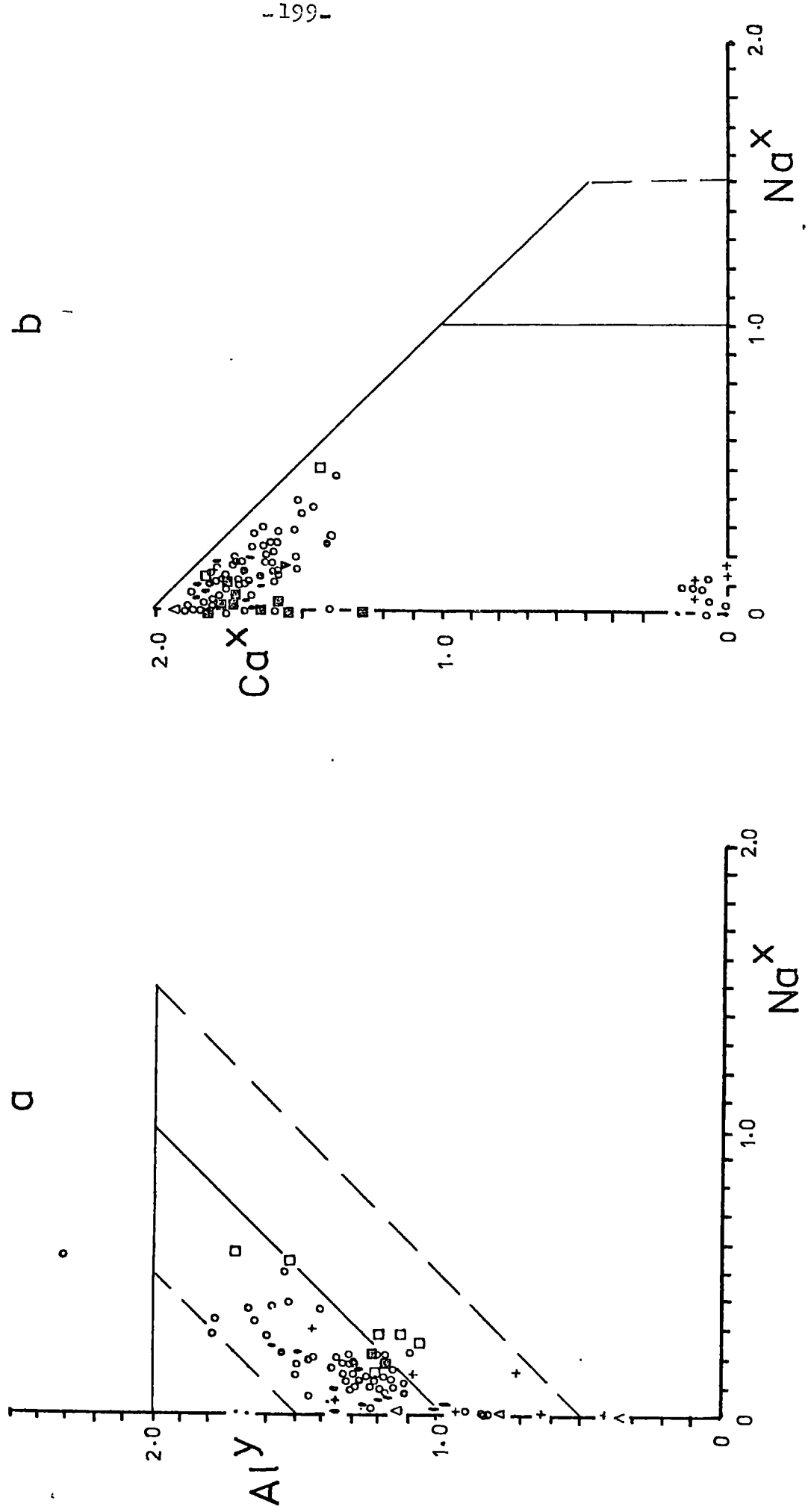
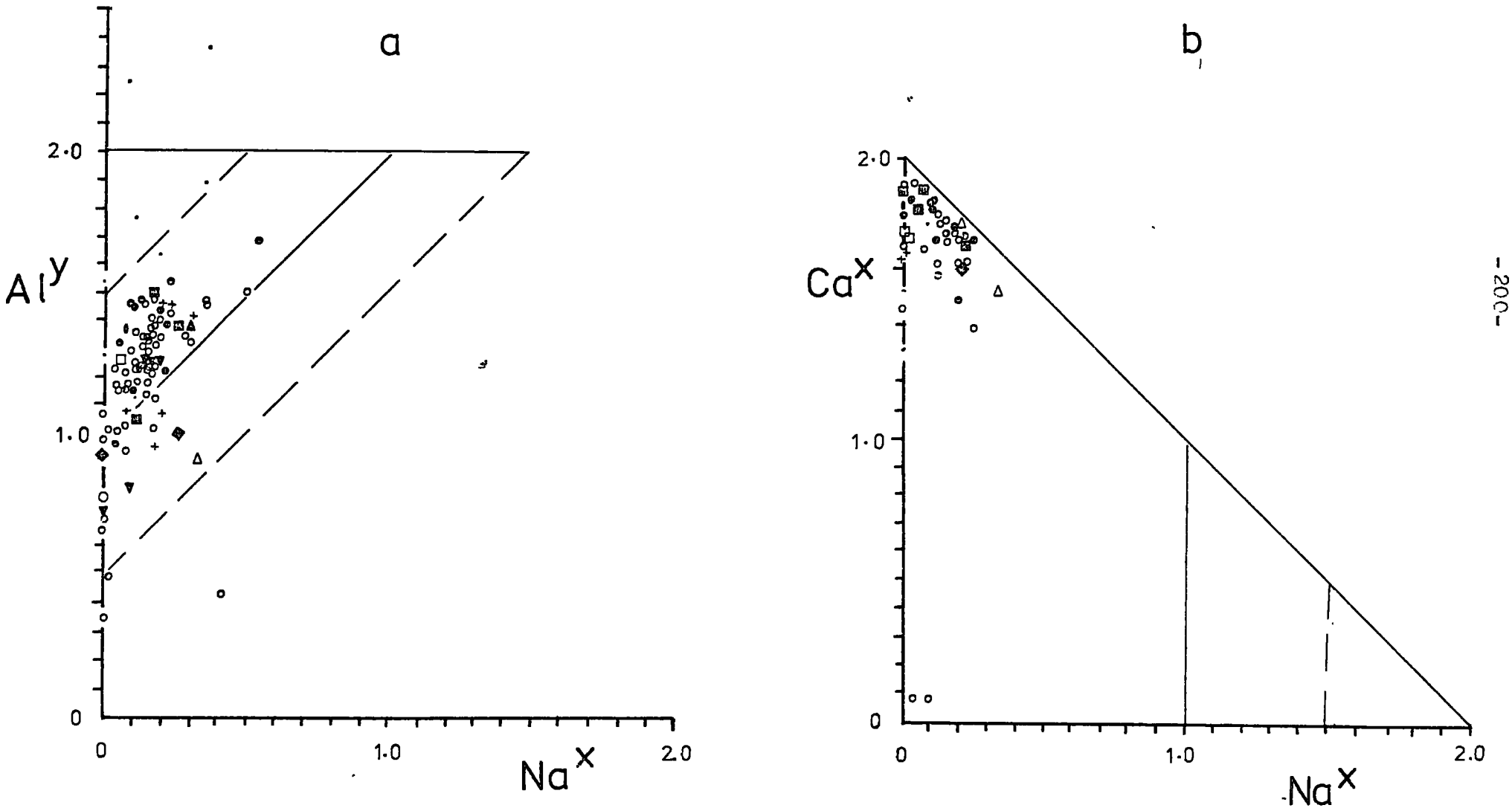


Fig. 7.13. Al^z 1.5—2.0, (Mg,Al^{vi})

Fig. 7.14. Al^{Z} 1.5 2.0 .(Mg,Fe^{3+})



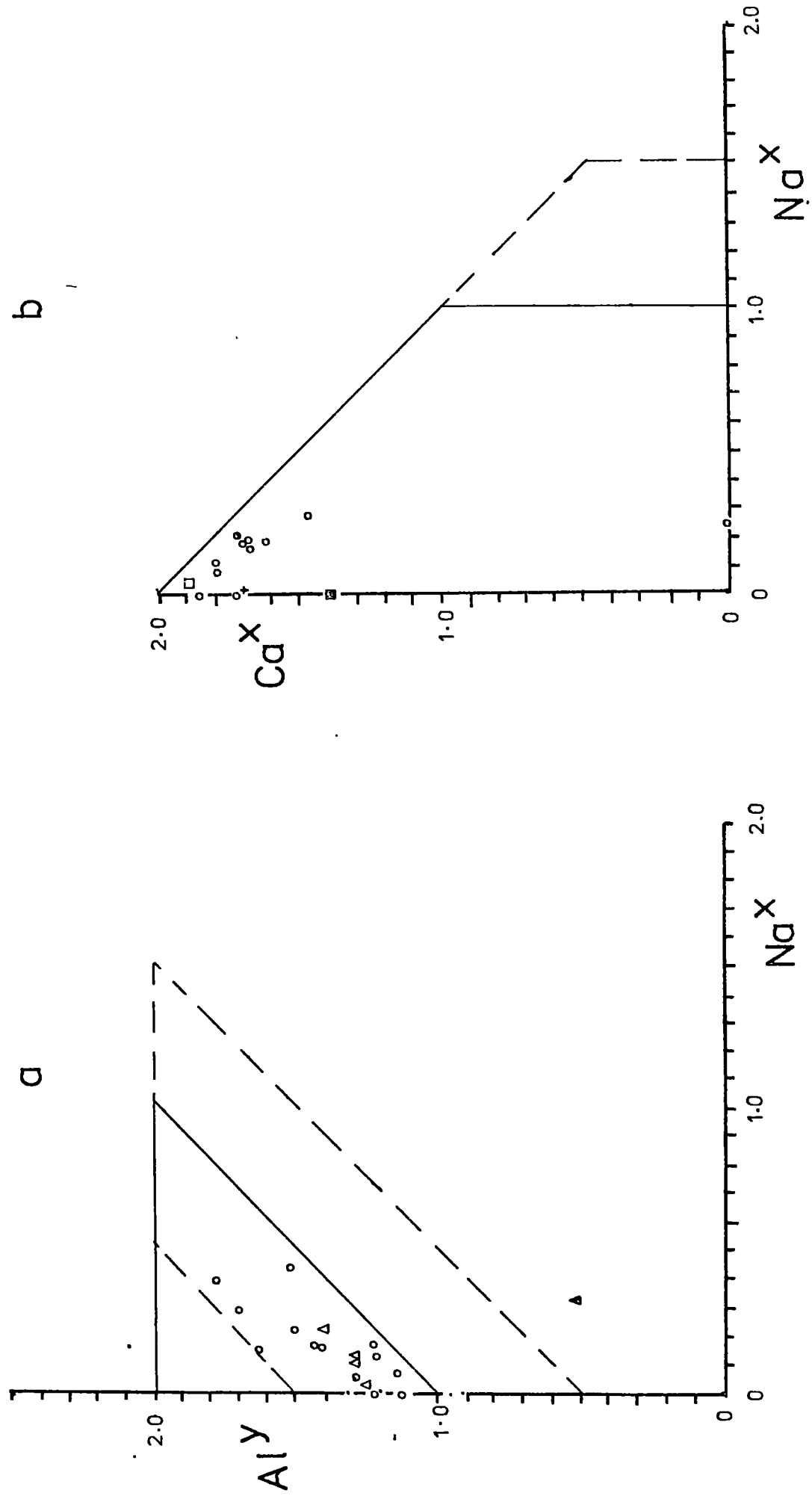


Fig. 7.15. Al^z 1.5—2.0, (Fe^{2+},Al^{vi})

Fig. 7.16. Al^{z} 1.5 – 2.0 , (Fe^{2+}, Fe^{3+})

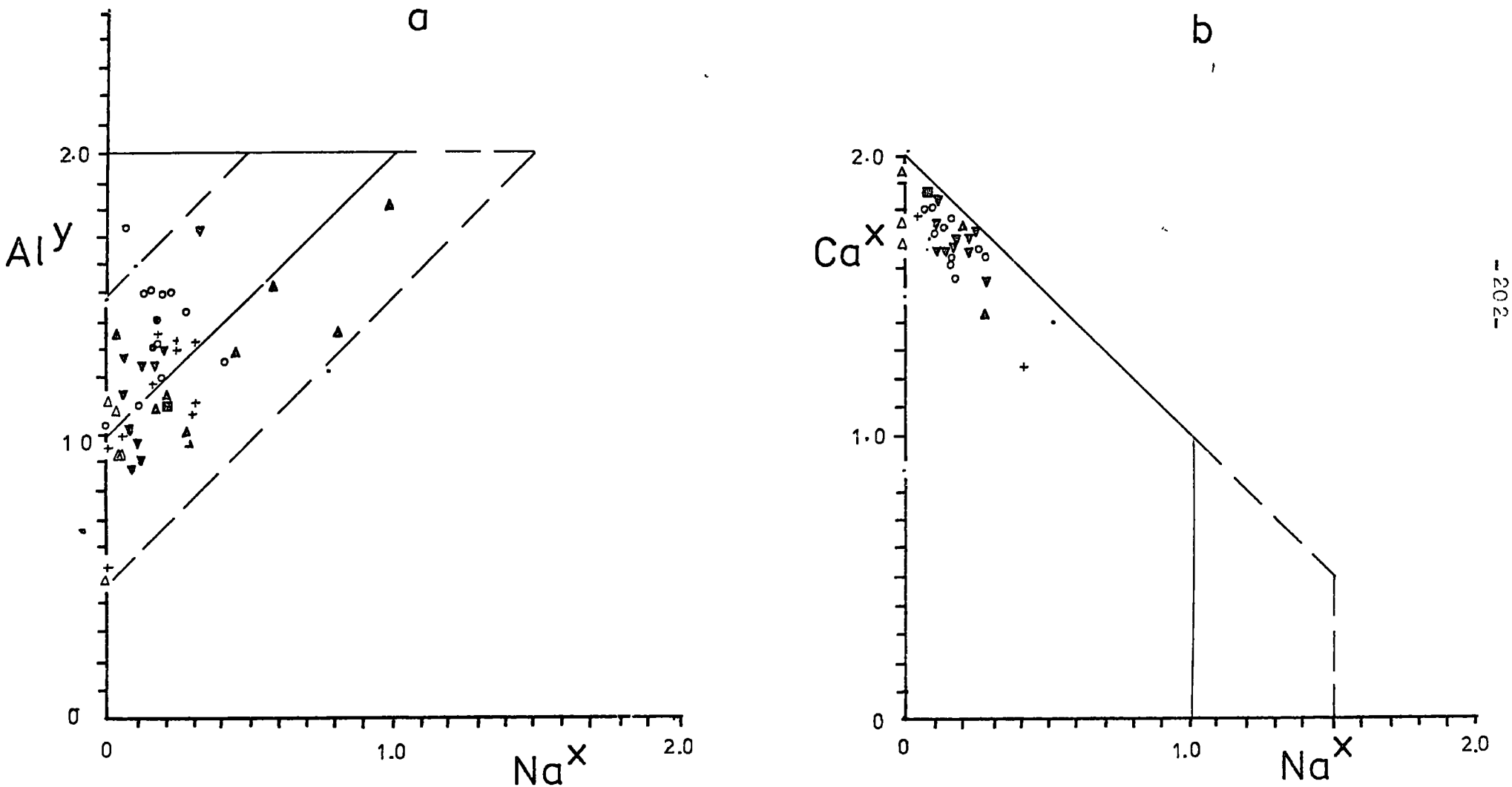


Fig. 7.17. Al^{z} 2.0 – 2.5, (Mg, Al^{vi})

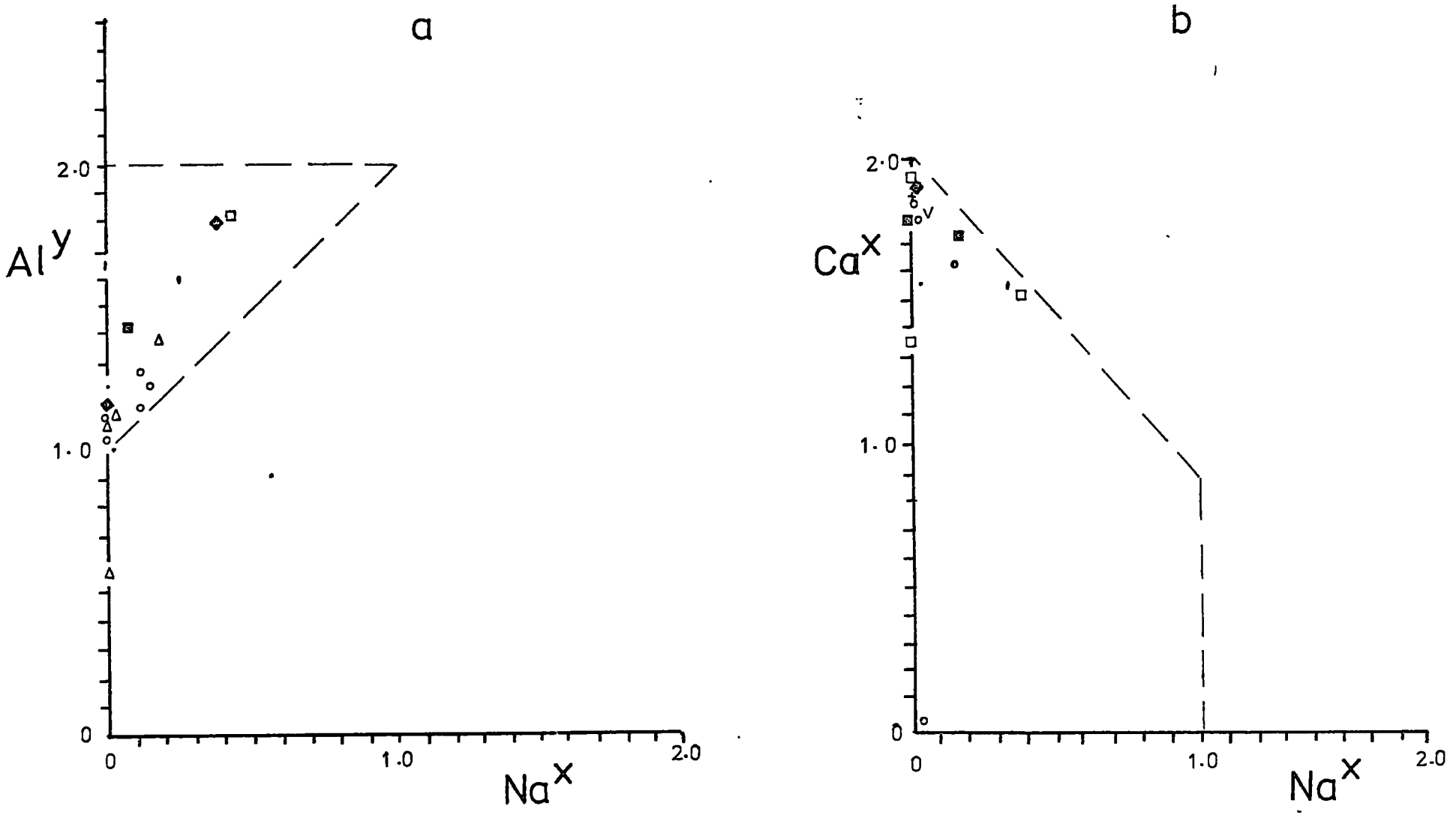


Fig. 7.18. Al^z 2.0—2.5 , (Mg,Fe^{3+})

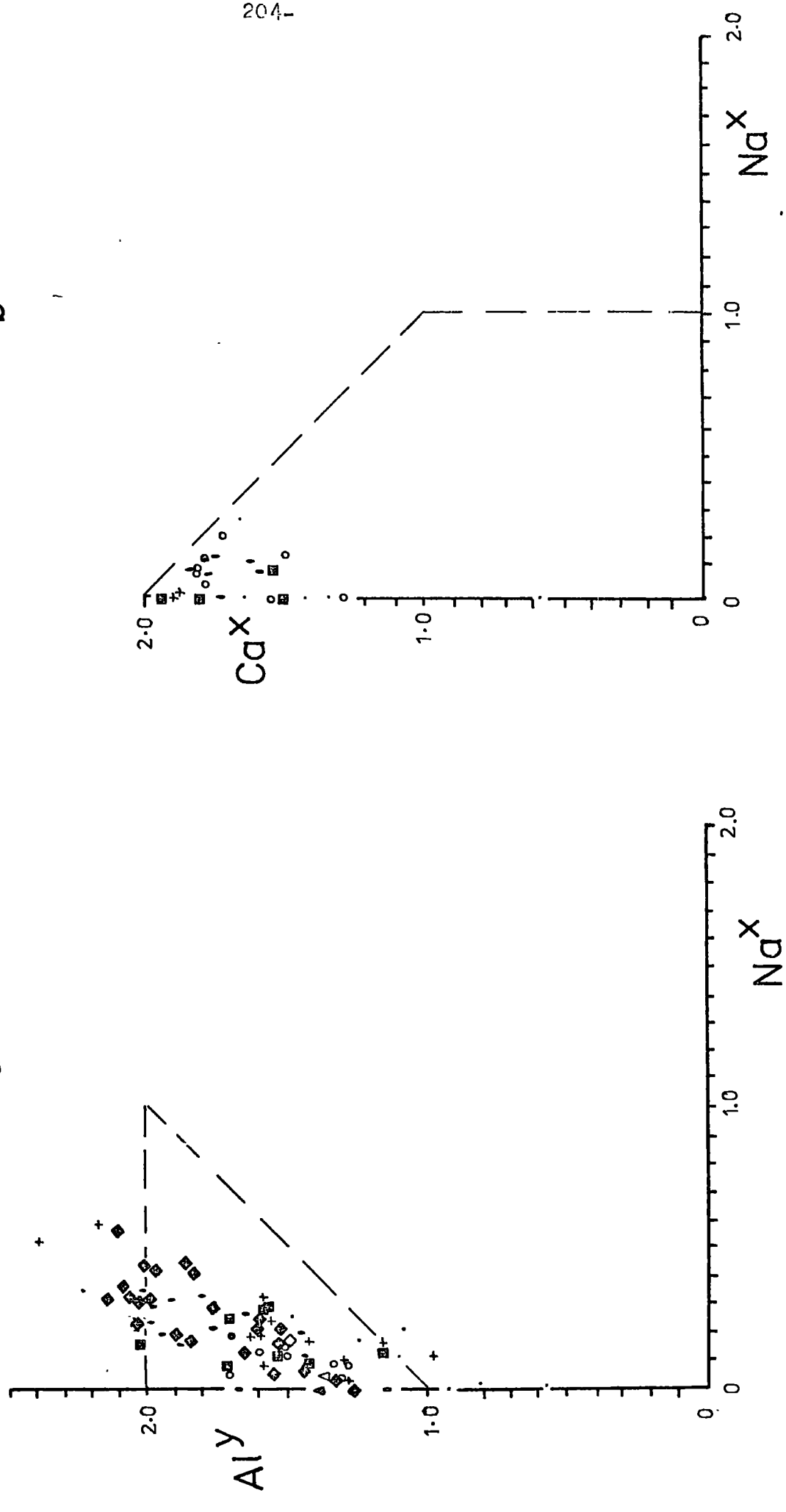
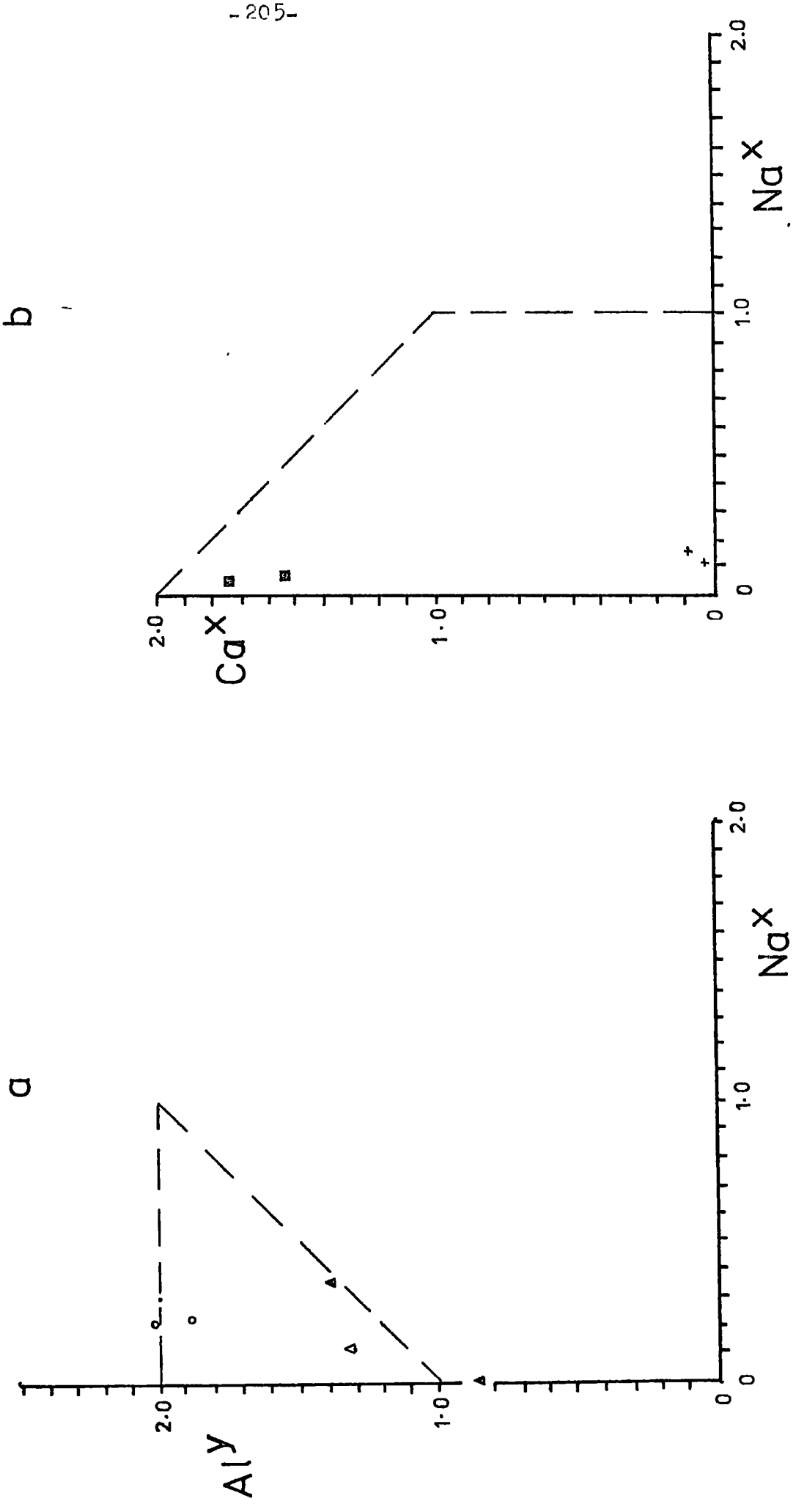


Fig. 7.19. Al^z 2.0—2.5, (Fe^{2+},Al^{vi})



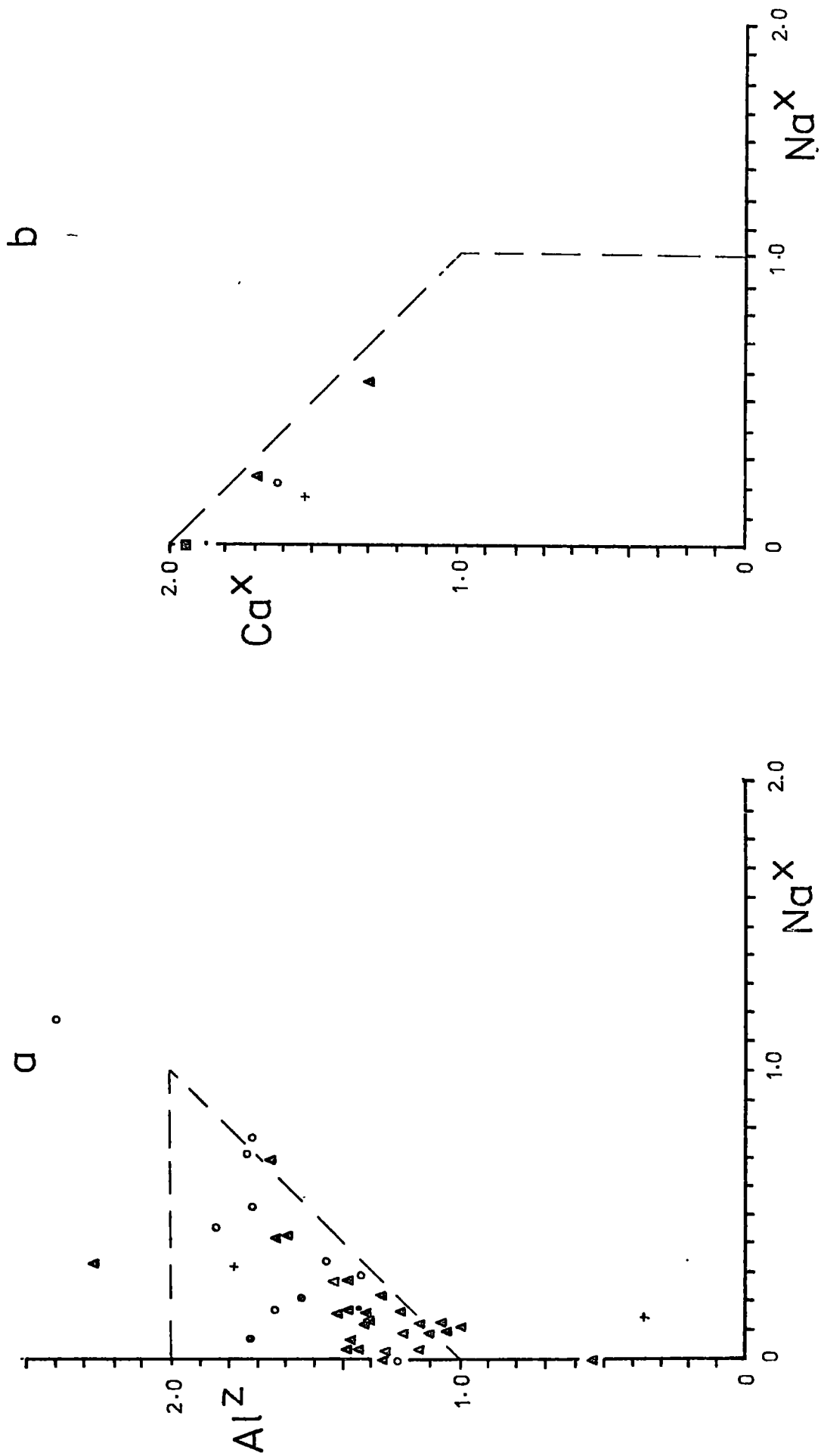


Fig. 7.20. Al^Z 2.0—2.5 , (Fe^{2+},Fe^{3+})

Figs. 7.21, 7.22. Al^Z versus Al^Y for basic atomic formulae in amphibole compositional space with $Na^X \leqslant 0.66$. Substitution in the basic atomic formula is as follows:-

7.21a. (Mg^{2+}, Al^{vi})

7.21b. (Mg^{2+}, Fe^{3+})

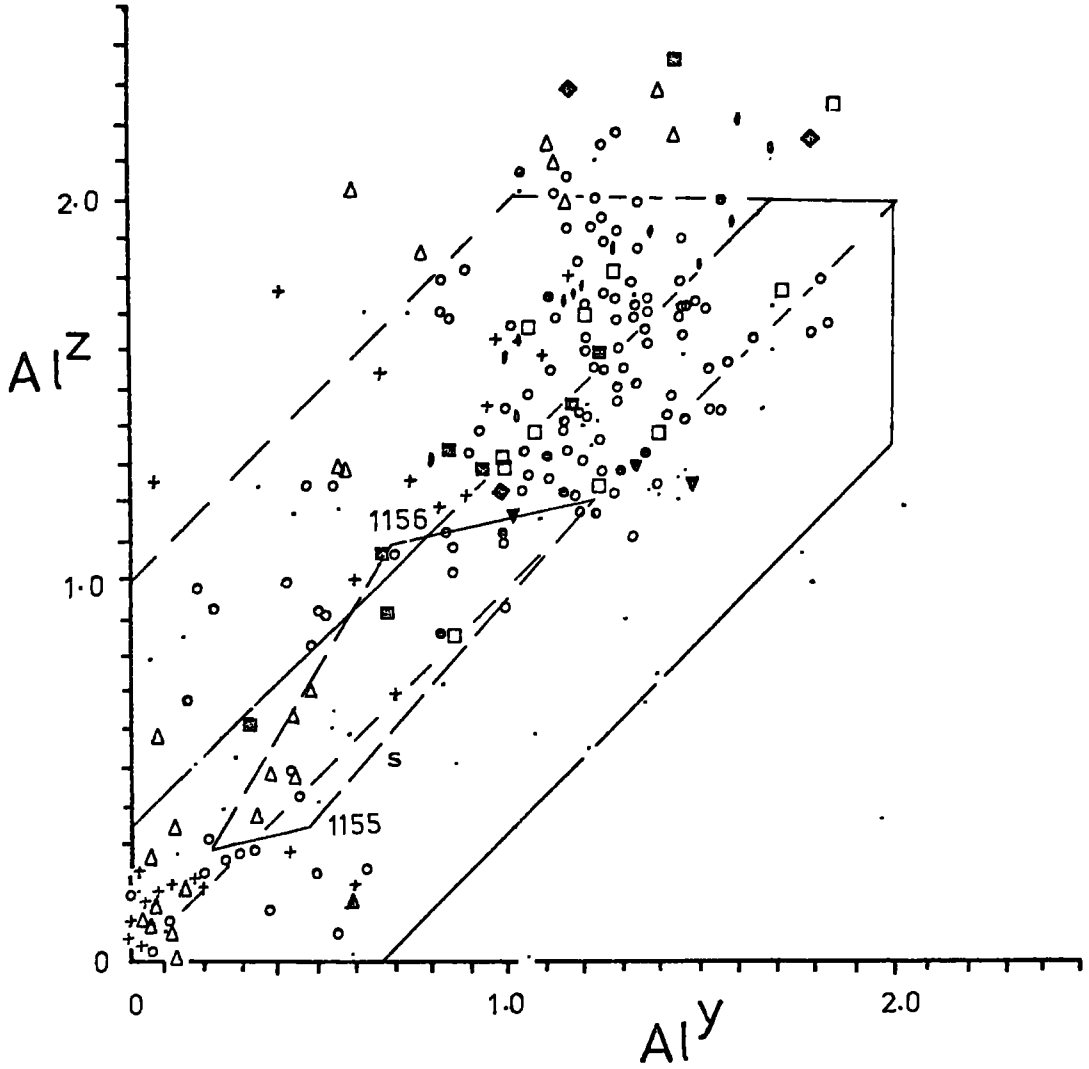
7.22a. (Fe^{2+}, Al^{vi})

7.22b. (Fe^{2+}, Fe^{2+})

Symbols are described in the text. The short bars on Fig 7.21a indicate the range of basic atomic formulae for the apparently co-existing pair of electron microprobe analyses 1155 - 1156, see Section 7.2.1. The solid and broken lines outline the limits of amphibole compositional space with $Na^X = 0.0$, and Na^X 0.66 respectively.

Fig. 7.21.

a. (Mg,Al^{vi})



b. (Mg,Fe^{3+})

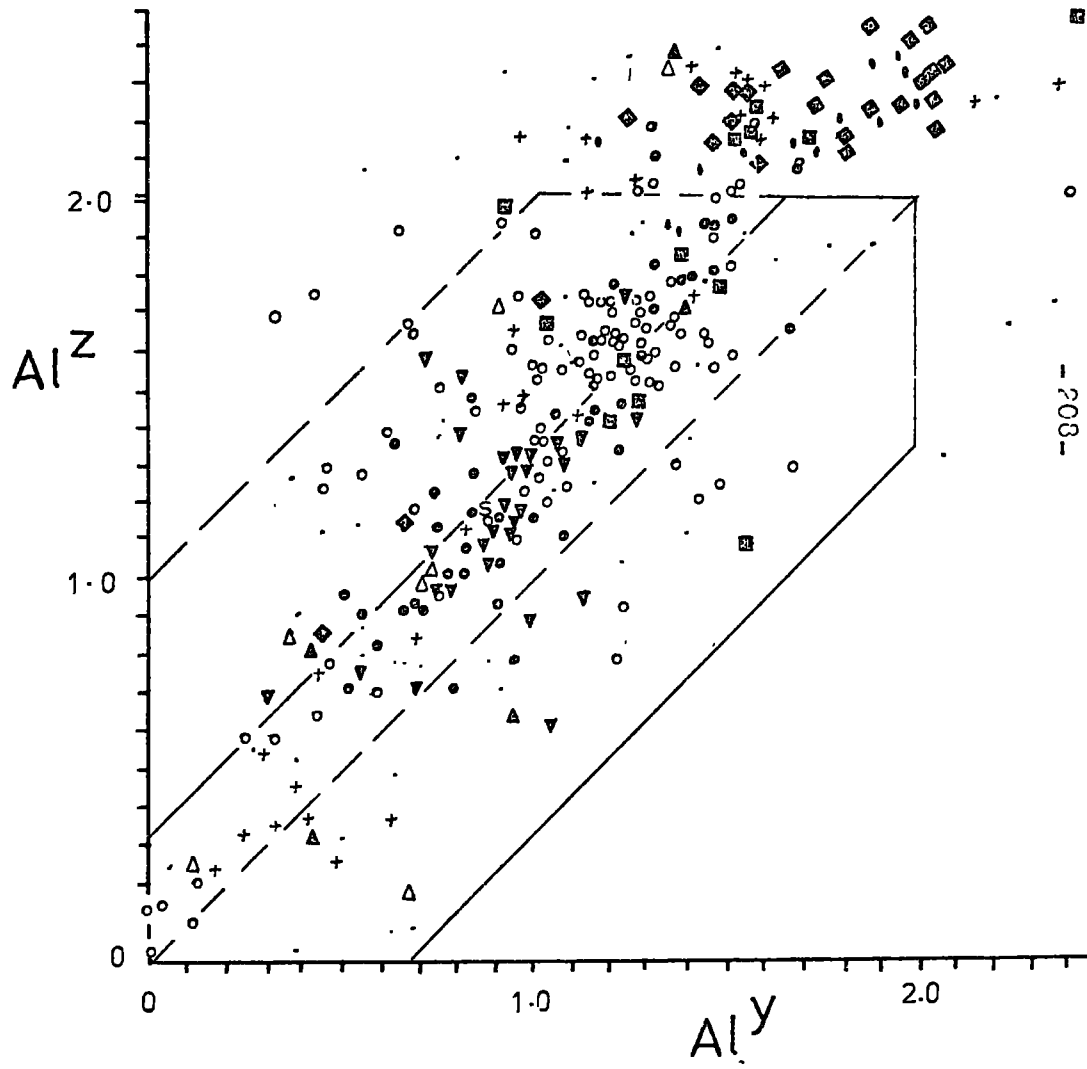
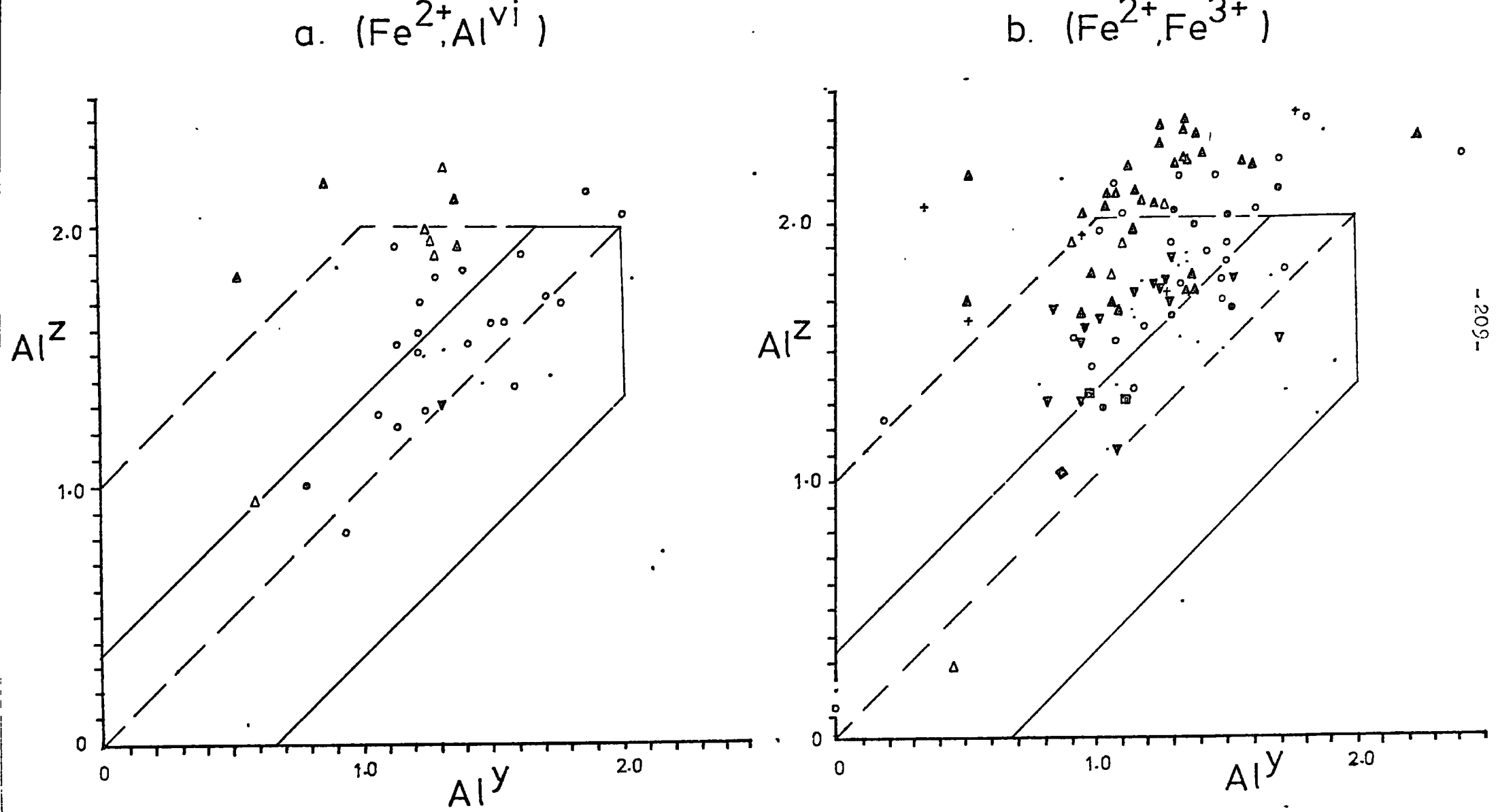


Fig. 7.22.



Figs. 7.23, 7.24. Al^{Z} versus Ca^{X} for basic atomic formulae in extended amphibole compositional space with $Na^{X} \leqslant 0.66$. Substitution in the atomic formulae is as follows:-

7.23a (Mg^{2+} Al^{vi})
7.23b (Mg^{2+} Fe^{3+})
7.24a (Fe^{2+} Al^{vi})
7.24b (Fe^{2+} Fe^{3+})

Symbols are described in the text. The solid lines represent the boundary of extended amphibole compositional space.

Fig. 7.23.

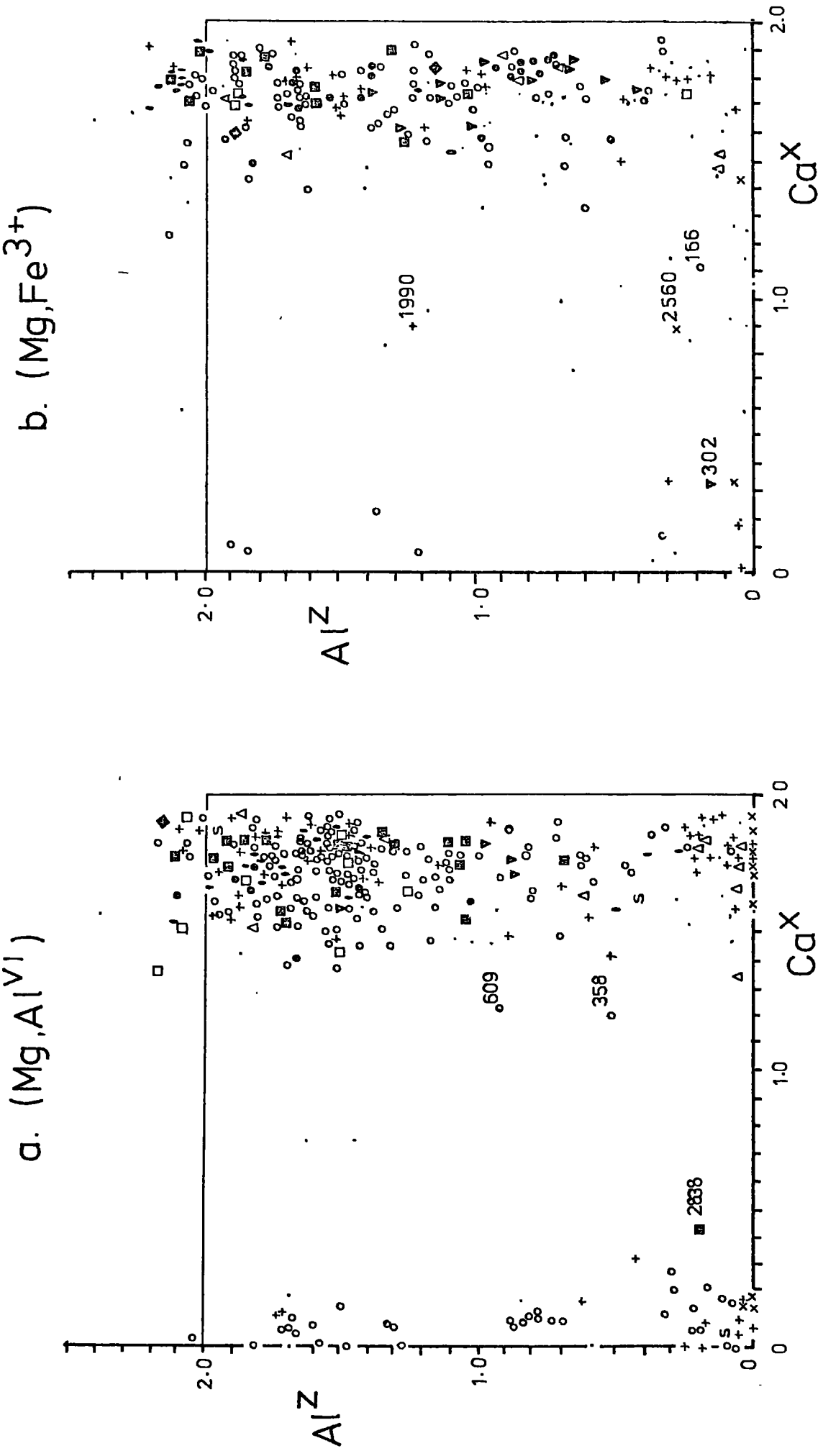
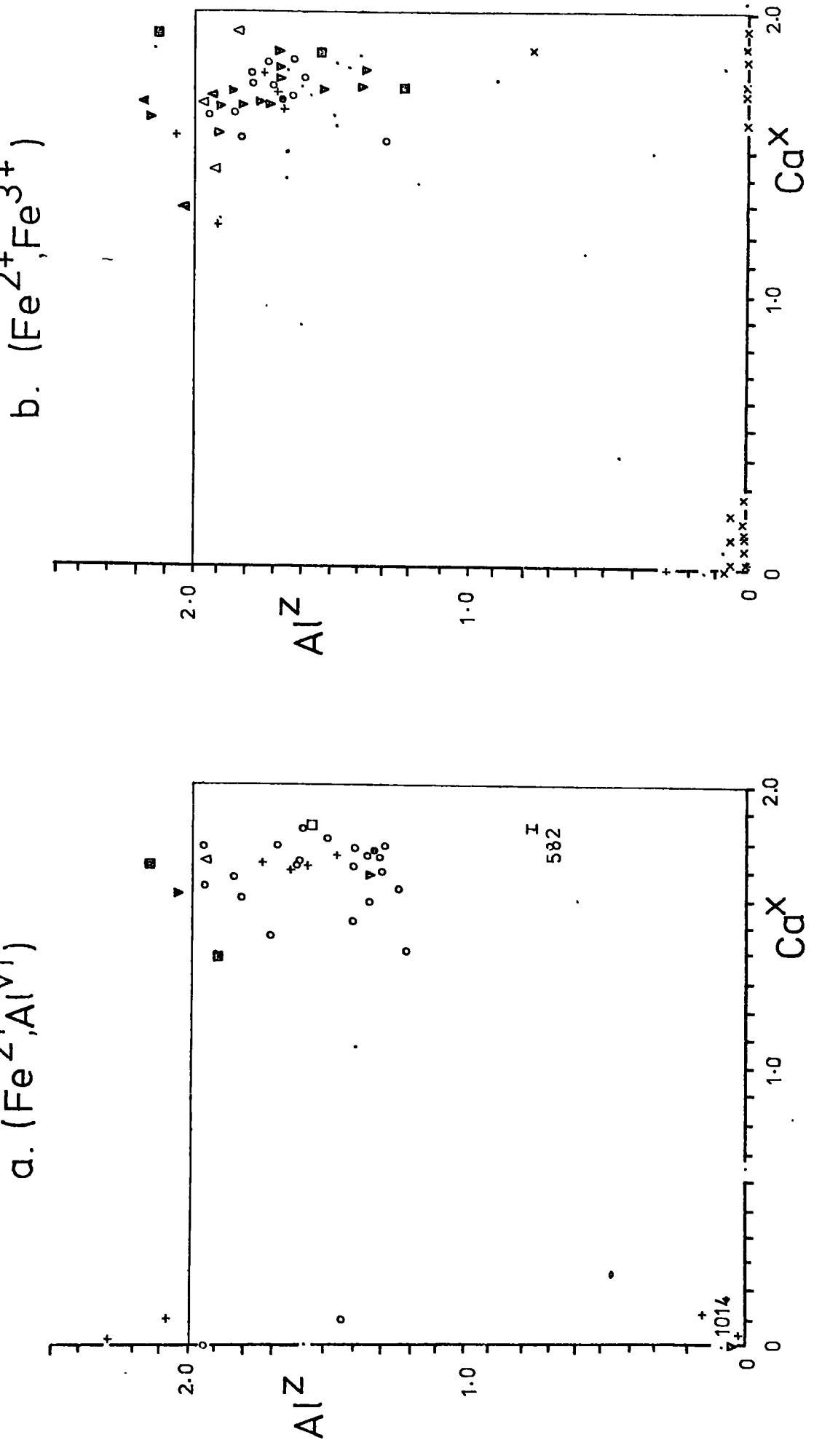


Fig. 7.24.



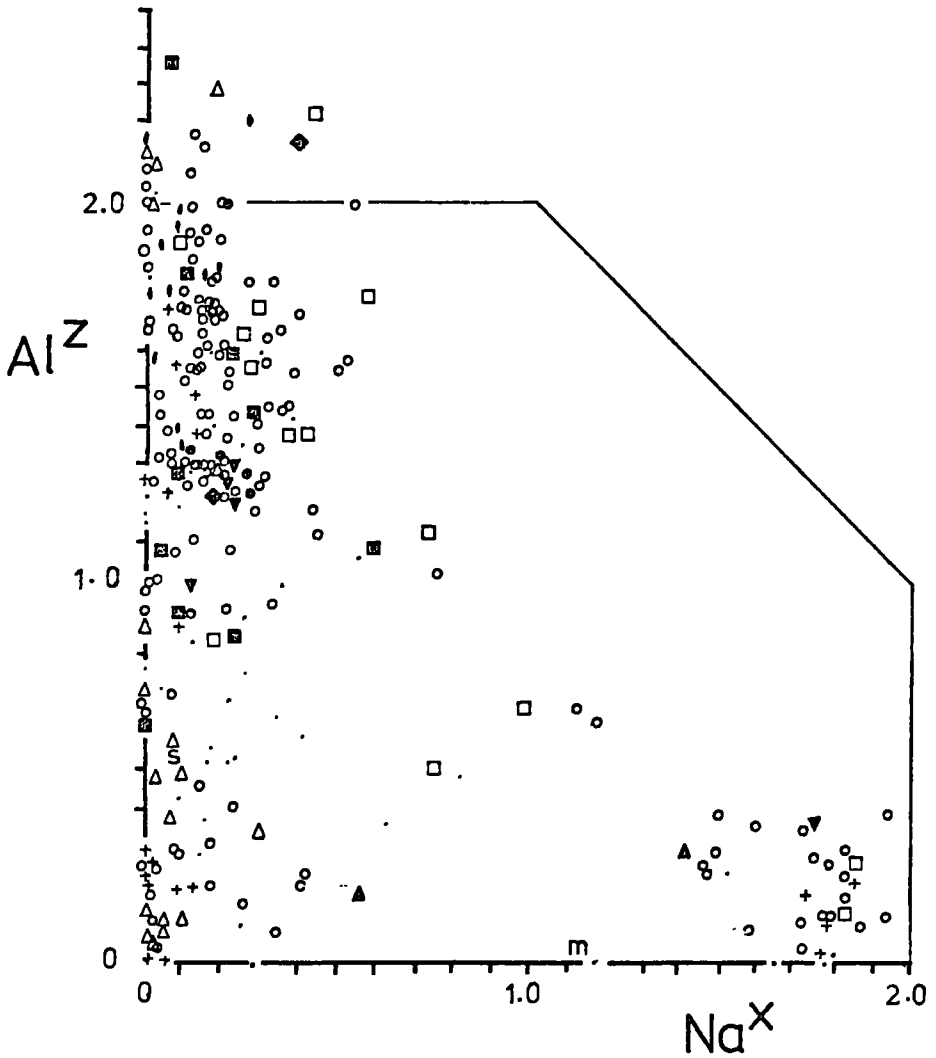
Figs. 7.25, 7.26. Al^{Z} versus Na^{X} for basic atomic formulae in amphibole compositional space. Substitution in the atomic formulae are as follows:-

7.25a	(Mg^{2+}, Al^{vi})
7.25b	(Mg^{2+}, Fe^{3+})
7.26a	(Fe^{2+}, Al^{vi})
7.26b	(Fe^{2+}, Fe^{3+})

Symbols are described in the text. The solid line indicates the boundary of amphibole compositional space.

Fig. 7.25.

a. (Mg,Al^{vi})



b. (Mg,Fe^{3+})

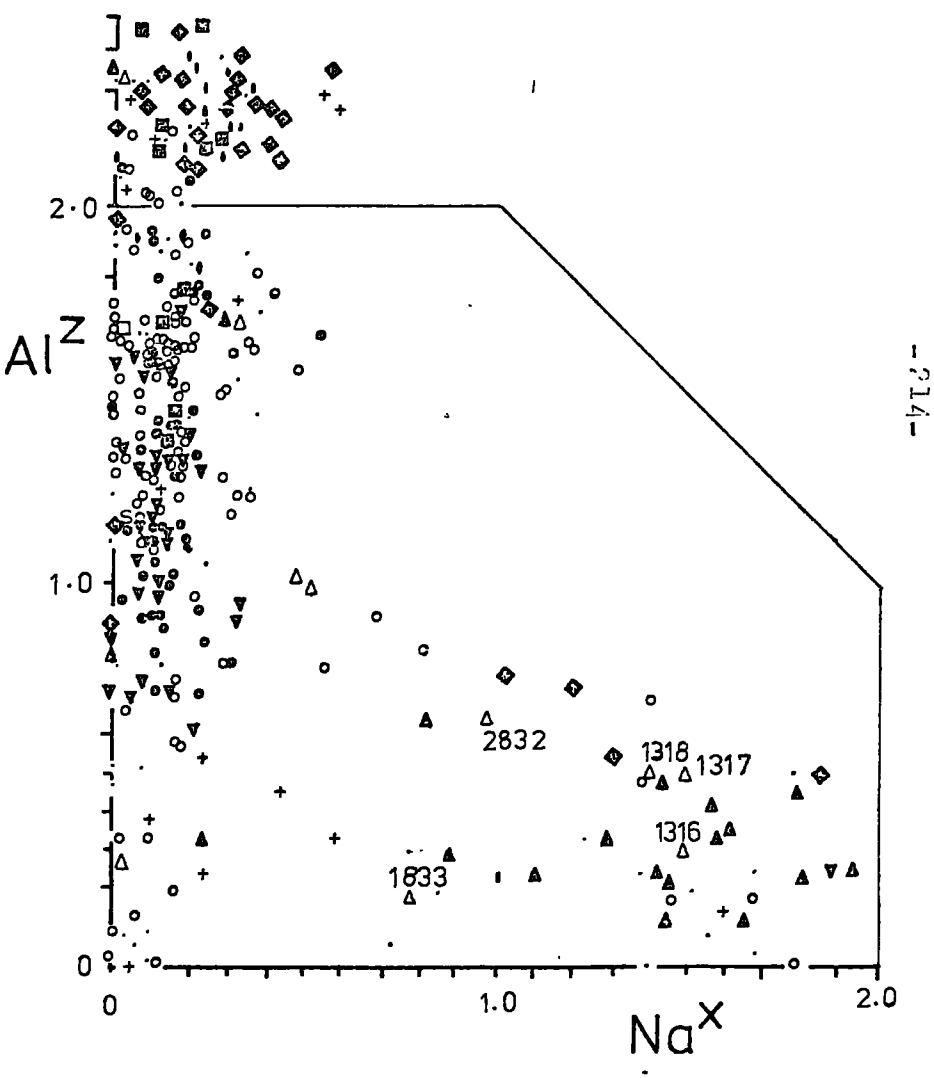
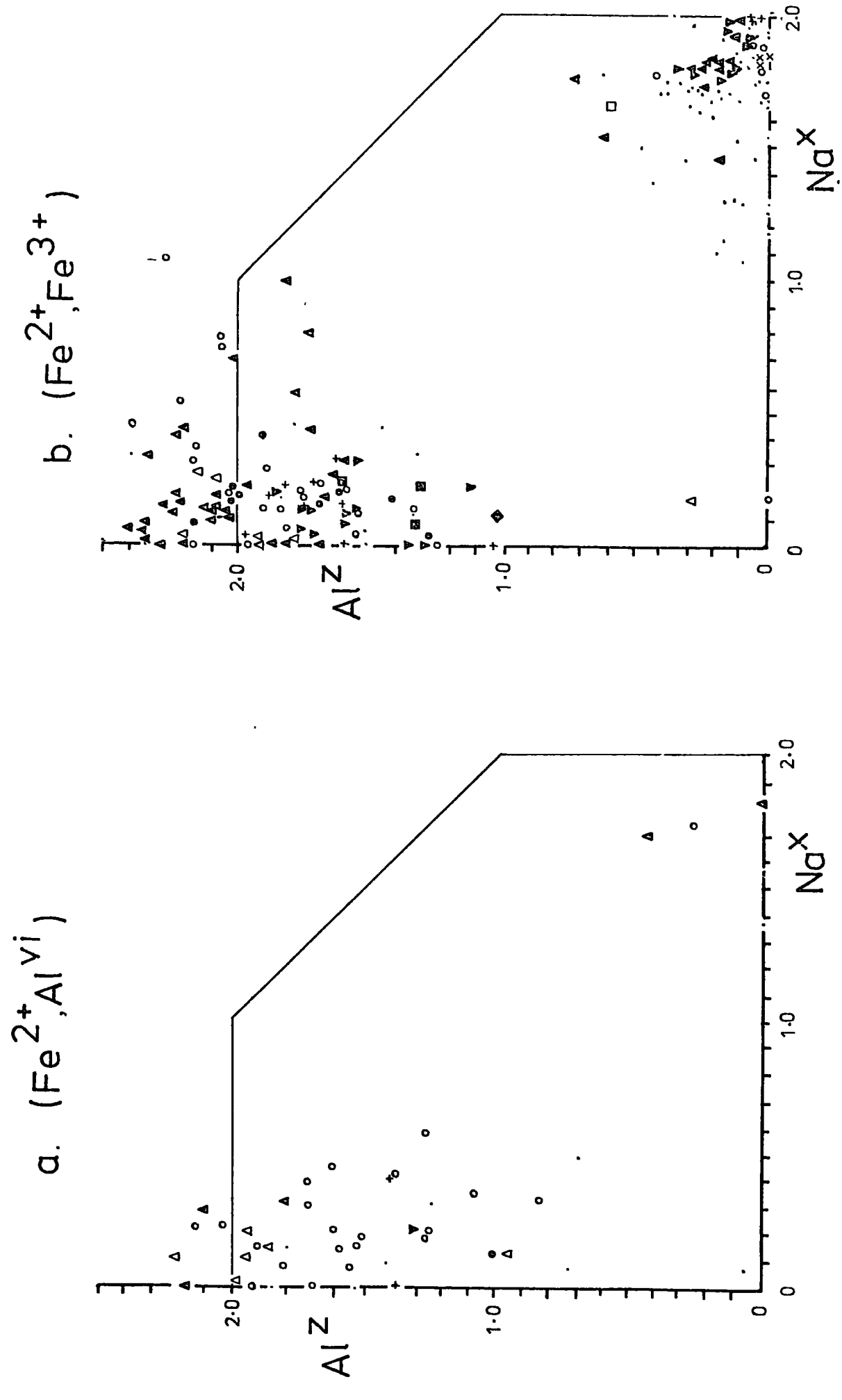


Fig. 7.26.



Figs. 7.27, 7.28. Al^Z versus Al^Y for basic atomic formulae in extended amphibole compositional space with $Mg^X > 1.33$, $Na^X \leqslant 0.66$. Substitution in the atomic formulae is as follows:-

7.27a. (Mg^{2+}, Al^{vi})
7.27b. (Mg^{2+}, Fe^{3+})
7.28a. (Fe^{2+}, Al^{vi})
7.28b. (Fe^{2+}, Fe^{3+})

Symbols are described in the text. The solid line is the limit of balanced basic atomic formulae with $Na^X = 0.0$.

Fig. 7.27.

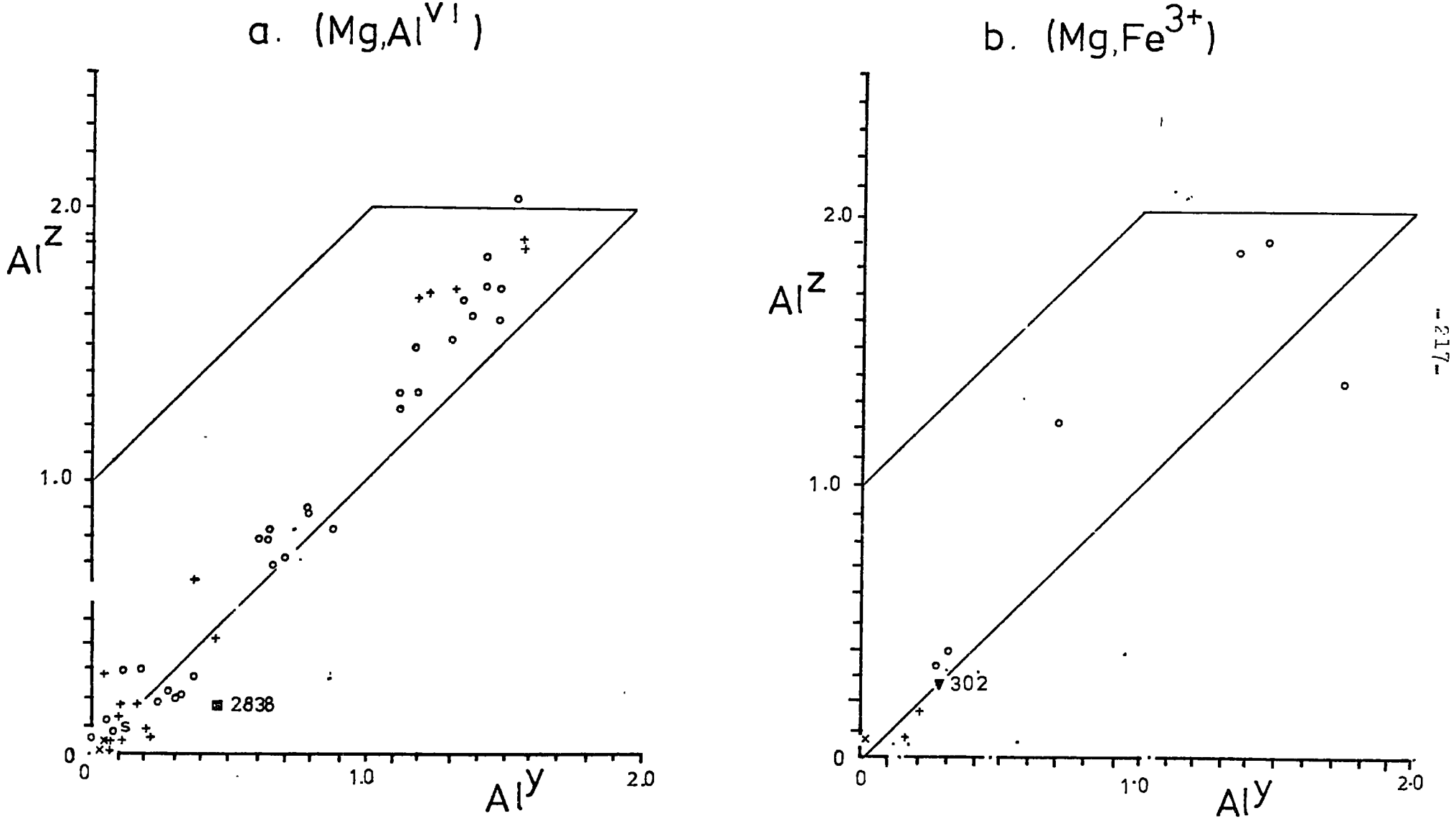
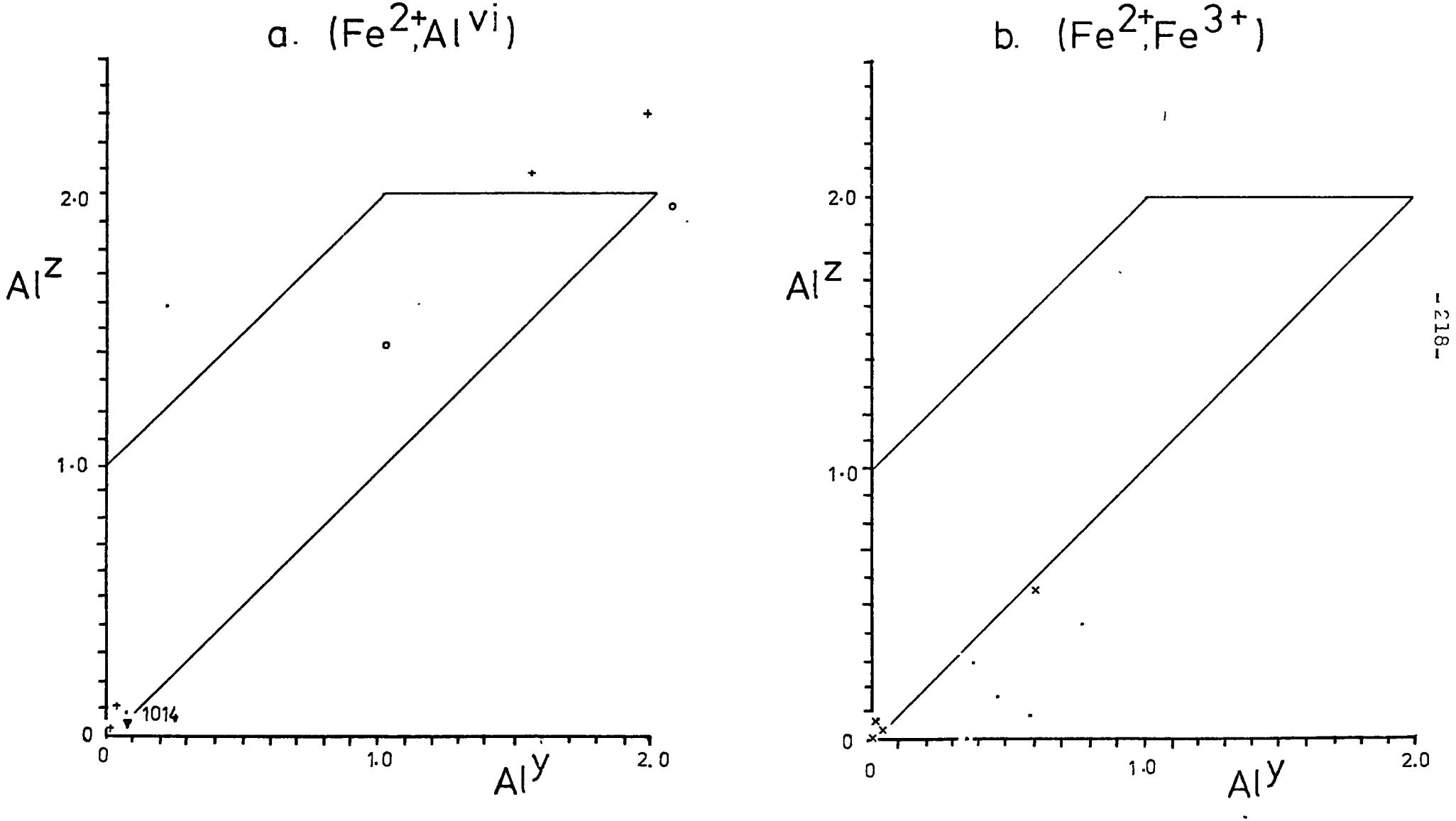


Fig. 7.28.



1.4 ($Ca + Na^X$ 1.6 - 0.6) separates the FeMgMn from the calciferous and alkali amphiboles. Only four analyses, 358 (Callegari & Monese 1971), 609 (Eskola 1914), 1990 (Schubert 1969) and 2102 (Weibull 1896) may be considered as intermediate. Of these 2102 with no CaO reported must be considered inferior and according to Leake (1968) 358 is probably impure. The purity of the remaining analyses is not known. Analyses, 166 and 2560 appear intermediate on Fig. 7.23b but this is on account of their high Na^X content, see Fig. 7.2b.

The major compositional break between the FeMgMn and the calciferous and alkali amphiboles is consistent with what is known of relevant miscibility relations. From experimental studies Cameron (1971) demonstrated a two amphibole region between cummingtonite and tremolite and exsolution textures in natural amphiboles have been reported for host and lamellae of P or C cummingtonite and tremolite or actinolite, P or C cummingtonite and 'hornblende', P cummingtonite and so called 'riebeckite - tremolite'. (Ross, Papike & Shaw 1969) and between Mn cummingtonite and magnesio-arfvedsonite (Robinson, Jaffe, Ross & Klein 1971). The analysis of host plus cummingtonite lamellae of the 'riebeckite - tremolite', 2560 (Klein 1966) is shown on Fig 7.2b where it plots near richterite. In addition, the apparently stable coexistence of separate grains of gedrite and hornblende (Stout 1971), anthophyllite and 'calcium amphibole' (Robinson, Ross & Jaffe 1971; Stout 1972) probably indicate further miscibility relationships.

Considering the FeMgMn amphiboles in greater detail, Figs 7.27, 7.28 show that these amphiboles lie in a narrow almost straight band extending from Anth. to Gd_{50} Na - Gd_{50}. Thus the coupled substitutions of Al^y Al^z for Mg^y Si (Anth - Gd) and Na^A Al^z for $\square$ Si (vertical on Figs 7.27, 7.28) are the most important in the basic atomic formulae of natural FeMgMn amphiboles. There is a hiatus in

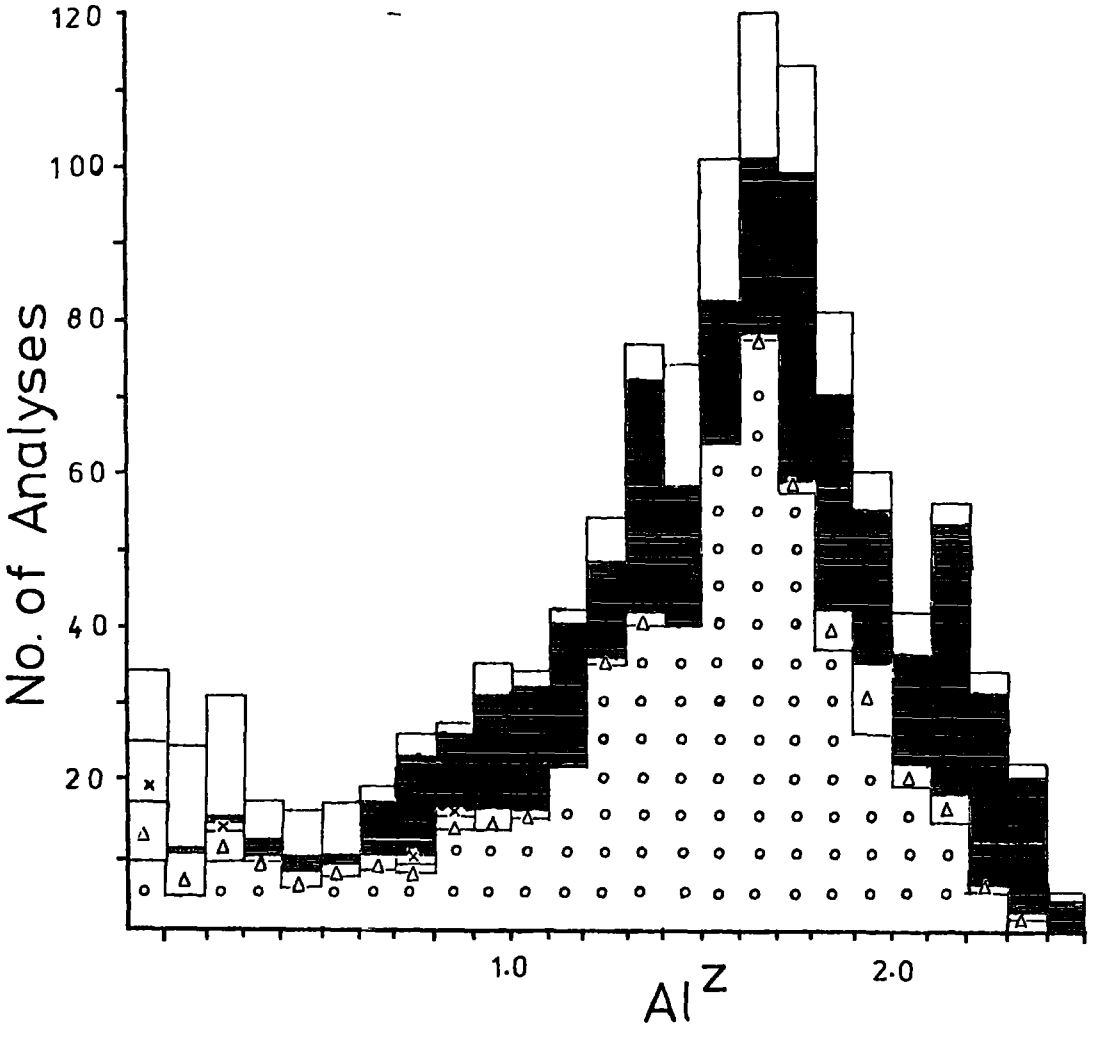
the basic atomic formulae near Al^Z 1.0 and this may be connected with reports of exsolution between gedrite and anthophyllite (Ross, Papike & Shaw 1969; Robinson Ross & Jaffe 1971). Substitutions $\square Al^Y = Na^A Mg^Y$ (horizontal on Figs 7.27, 7.28) and those involving Na^X are less important when describing natural FeMgMn amphiboles. Robinson, Ross & Jaffe (1971) described an almost identical variation for a different collection of analyses including analyses not in the amphibole data file and Rabbit (1948) noted a gap between low and high Al_2O_3 orthoamphiboles.

Within the calciferous and alkali amphiboles in A.C.S. and the adjacent portion of E.A.C.S. analyses are concentrated in two regions, one with Na^X less than 0.6 and the other with Na^X greater than 1.3 separated by an intermediate region in which analyses are less numerous. The majority of all amphiboles plot in a zone extending from Na^X 0.0 - 0.6 parallel to the Tr - Ed - Pa - Ts face of A.C.S. and extending into E.A.C.S. up to approximately Mg^X 0.6 ($Ca + Na^X$ 1.4). Within this zone natural amphiboles lie in a broad band between ($Tr_{50}Ed_{50}$) - Pa and Tr - Ts but amphiboles close to the vertices Ed and Ts are uncommon. Just as in the FeMgMn amphiboles, the most important coupled substitutions in the basic atomic formulae of these calcium rich amphiboles involve $Al^Y Al^Z = Mg^Y Si$ (Tr - Ts on Figs 7.21, 7.22) and $Na^A Al^Z = Si$ (vertical on Figs 7.21, 7.22) with $\square Al^Y = Na^A Mg^Y$ (horizontal) increasing in importance relative to the FeMgMn amphiboles. Principal components analysis of Leake's (1968) collection by Saxena & Ekström (1970) also showed the importance of these three coupled substitutions in the calciferous and subcalciferous amphiboles. A number (160 or approximately 8 per cent) of basic atomic formulae, in particular from igneous and skarn parageneses, have Al^Z in excess of 2.0 up to an upper limit of 2.5. This can be seen from Fig 7.29 which is a histogram of the Al^Z content of those

Fig. 7.29 Histogram of Al^Z in basic atomic formulae with $Na^X \leqslant 0.66$ and $Mg^X \leqslant 0.66$ calculated to 23(O) for those analyses in the amphibole data file with either H_2O+, F or Cl determined.

Symbols are as follows:-

- [O] metamorphic, host rocks excluding calcareous and ferruginous host rocks.
- [▒] igneous host rocks.
- [Δ] metamorphosed calcareous host rocks.
- [I] metamorphosed ferruginous host rocks.
- [ ] host rocks, not known.


120
100
80
60
40
20
No. of Analyses
1.0
2.0
Al Z

basic atomic formulae with $Na^X \leqslant 0.66$ and $Mg^X \leqslant 0.66$. It is apparent from Fig 7.29 that the calcium rich amphiboles display a bimodal distribution with respect to Al^Z with modes at 0.0 - 0.1 and 1.6 - 1.7 and a minimum at 0.4 - 0.5. Leake (1962) observed a similar bimodal distribution with a minimum at Si^{4+} 7.1 - 7.3 (Al^Z 0.7 - 0.9) in a collection of calciferous ($Ca^{2+} > 1.5$) and subcalciferous ($1.0 < Ca^{2+} < 1.5$) amphiboles from various parageneses. However it is a noteworthy feature of Fig 7.29 that the bimodal distribution is not due to the sum of individual bimodal distributions in each paragenesis. Only amphiboles from calcareous metamorphic rocks display a bimodal distribution. Amphiboles from general metamorphic and igneous parageneses are unimodally distributed. The low Al^Z mode is due to amphiboles from calcareous, ferruginous and to a lesser extent unknown parageneses. The significance of this will be dealt with further in Section 7.2.1 when possible gaps in A.C.S. will be discussed.

A third concentration of basic atomic formulae occurs with $Na^X > 1.3$ and extends between the vertices G and Ec (Figs 7.1, 7.2). These are almost exclusively confined to Al^Z less than 0.5 but see Section 5.4.1. Coupled substitutions in the basic atomic formulae which do not involve changes in Na^X are important, in particular $\square Al^Y = Na^A Mg^Y$ (G to Ec on Figs 7.1, 7.2).

Amphiboles with Na^X between 0.6 and 1.3 do occur but are not very numerous and indicate that coupled substitutions involving $Na^X = Ca$ are not very common. These intermediate amphiboles are of two types: (i) (Fe^{2+}, Fe^{3+}) substituted basic atomic formulae with Al^Z in excess of 1.5 which approach Su (Figs 7.16, 7.20, 7.26) and (ii) (Mg^{2+}, Fe^{3+}) and less common (Mg^{2+},Al^{vi}) substituted basic atomic formulae with Al^Z less than approximately 1.0 (Figs 7.1, 7.2, 7.5, 7.6, 7.25).

From the observed distribution of analyses in A.C.S. it is apparent that Phillips' two fold subdivision at Na^X 1.0 into the calciferous and alkali amphiboles fails to emphasise the numerical superiority of basic atomic formulae with Na^X less than 0.6 or greater than 1.3 and the relative scarcity of intermediate amphiboles. It is suggested that a three fold subdivision of amphibole compositional space should be adopted with boundaries at Na^X 0.66 and 1.33. Amphiboles belonging to each of these groups may be designated calcic, soda calcic and alkali respectively. Neither of these boundaries coincides with those of sensu dominante nomenclature but this would be true of any boundary parallel to the Al^Z and Al^Y axes. Extended amphibole compositional space may be subdivided in a similar manner consistent with the observed distribution of amphiboles by using boundaries at Mg^X 0.66 (Ca + Na^X 1.33) and Mg^X 1.33 (Ca + Na^X 0.66) parallel to the Al^Z axis. That portion of E.A.C.S. with $Mg^X \leqslant 0.66$ can be further subdivided into calcic, soda calcic and alkali amphiboles by extending the boundaries of A.C.S. into E.A.C.S. Therefore the following definitions of the calcic, soda calcic and alkali amphiboles are suggested: -

calcic, basic atomic formulae with $Na^X \leqslant 0.66$ and $Mg^X \leqslant 0.66$.

soda calcic, basic atomic formulae with Na^X 0.66 - 1.33 and $Mg^X \leqslant 0.66$

alkali, basic atomic formulae with $Na^X \geqslant 1.33$.

Those amphiboles with $Mg^X \geqslant 1.33$ may be termed the FeMgMn amphiboles. No satisfactory term could be found for those amphiboles (if any really exist) with Mg^X 0.66 - 1.33. In Chapter 5 it was noted that the concept of the basic atomic formula could be extended to all amphiboles by incorporating Fe^{2+}, Mg^{2+}, Mn^{2+} in X as Ca, Li^+ in X as Na^X and Li^+ in A as Na^A. By doing this all amphiboles can be made to plot in amphibole compositional space and by consulting Table 5.1 can be given a sensu dominante name. Obviously the sensu dominante name is of

little revelance for amphiboles with extensive Mg^X substitution. However it is suggested that sensu dominante nomenclature is of value if applied to the calcic, soda calcic and alkali amphiboles, that is to those amphiboles with Mg^X less than 0.66. The nomenclature derived from the observed distribution of natural amphiboles and the sensu dominante nomenclature will be used throughout the remainder of this work.

7.2. Possible miscibility relations within the calcic, soda calcic and alkali amphiboles.

In Section 7.1 it was noted that basic atomic formulae of calcic, soda calcic and alkali amphiboles were not equally distributed over A.C.S. and the adjacent portion of E.A.C.S. Soda calcic amphiboles are uncommon compared with calcic and alkali amphiboles and calcic amphiboles with Al^Z about 0.5 were less common than those with higher and lower Al^Z. This might be attributed to sampling bias but this seems unlikely since Sundius (1946), Deer, Howie & Zussman (1963) and Ernst (1968) have each remarked on the scarcity of soda calcic amphiboles and in addition to Leake (1962), Read (1973) reported a gap in electron microprobe analyses from Central and Western Otago between Al^Z 0.6 - 0.9 (Na^X 0.0) which 'narrowed and eventually disappeared' at Al^Z 0.7 (Na^X 0.4), Graham (1974) found a gap at Si^{4+} 7.0 (Al^Z 1.0) in electron micrprobe analyses from Dalradian epidiorites, and Kostyak & Sabolev (1969) found a minimum in total Al^{3+} at 1.0 in metamorphic amphiboles.

Three general explanations have been advanced to explain one or both of these features, (i) the existence of a solvus or solvi (Sundius 1946; Boyd 1959; Ernst 1968), (ii) the composition of amphibole in equilibrium with chlorite in a metamorphic assemblage alters markedly with small changes in temperature or pressure

(Graham 1974), and (iii) the scarcity of analyses reflects the frequency of occurrence of appropriate conditions (Mottana & Edgar 1969).

It is beyond the scope of the present work and the content of the amphibole data file to investigate the latter two hypotheses in any detail. As far as the author is aware reports of exsolution textures in which both the host and exsolved phase are either calcic, soda calcic or alkali amphiboles (Klein 1969; Cooper & Lovering 1970; Cooper 1972) have not been confirmed. However, actinolite - glaucophane, hornblende - galucophane and actinolite - hornblende pairs have been reported by a considerable number of workers (for references to these see Ernst 1963 , 1968; Klein 1969; Cooper & Lovering 1970; Ernst et al. 1970; Graham 1974) and in this connection it seemed appropriate to compare the composition of amphibole pairs included in relation COEXISTENCE (Chapter 4, Appendix 9) with the observed distribution of basic atomic formulae. Such an approach will not prove the existence of a solvus, rather it will at best indicate whether two lines of evidence are consistent with such an interpretation. In order to restrict attention to amphiboles where equilibrium is most likely to have been achieved only those pairs in which the original description explicitly states that discrete grains were seen in contact and separated by optically and chemically sharp boundaries have been used. Where necessary optimum iron oxidation states have been calculated using the method outlined in Chapter 3.

7.2.1. Miscibility relations within the calcic amphiboles.

Petrographic observation of sharp, apparently non-gradational, contacts between actinolite and blue-green hornblende have been reported from rocks of the andalusite - sillimanite facies series (Miyashiro 1958; Shido 1958; Shido & Miyashiro 1959) and the kyanite - sillimanite facies series (Cooper & Lovering 1970; Graham 1974). The

change is commonly taken to indicate the transition between the greenschist and albite epidote amphibolite facies. Miyashiro (1958), Shido (1958) and Cooper & Lovering (1970) interpreted these an equilibrium features involving a solvus but Graham (1974) considered that non-equilibrium was more likely.

A search of relation COEXISTENCE located a number of calcic amphibole pairs but only one was in apparent equilibrium. These were the electron microprobe analyses 1155 - 1156 (Klein 1969 assemblage 2 - 1) from a hornblende actinolite rock, Tsintbolovolo, Madagascar. Optimum iron oxidation states were estimated for the pair and the ranges of possible basic atomic formulae are indicated by thick bars on Fig. 7.21a. The actual tie-line must lie somewhere within the quadrilateral outlined by linking the ends of the bars. In Fig. 7.21a and Figs 7.30 - 7.34, which follow, the lower left and upper right limits of the bars correspond to the highest and lowest reduced iron ratios consistent with a balanced basic atomic formula.

The separation of the basic atomic formulae of the pair with Al^z 0.30 - 0.36 and 1.08 - 1.21 corresponds closely with that portion of the calcic amphiboles where basic atomic formulae are not very numerous (Figs 7.21, 7.23, 7.29) and as such it is not inconsistent with the existence of a solvus. However, the fact that only one such pair was located, and Fig. 7.29 indicates a unimodal and not bimodal distribution of Al^z in amphiboles from non-calcareous parageneses, suggests that if a solvus does exist it must be either restricted by, or change location with, changes in physical and chemical conditions. Jasmund & Schafer (1972) synthesised an amphibole solid solution in the join Tr - Ts between Tr_{100} - $Tr_{45}Ts_{55}$ (Al^z 0.0 - 1.1) at 450 - 900° C and 2 kb. In addition Ernst (1972) reported an unbroken range of calcic amphiboles with respect to Al^z 'without exsolution lamellae, separate grains or armoring' from metabasics and metapelites in the

Sanbagawa (Outer) Metamorphic Belt, Shikoku, Japan which had been metamorphosed under conditions intermediate between the greenschist and glaucophane lawsonite schist facies up to the albite epidote amphibolite facies (Ernst et al. 1970; Ernst 1972). It is concluded that evidence for a solvus in the calcic amphiboles remains meagre and inconclusive.

7.2.2. Miscibility relations between the calcic and alkali amphiboles.

Turning now to a consideration of the relationship between the calcic and alkali amphiboles. In many instances where a calcic and alkali amphibole are found together textural evidence of non-equilibrium has been interpreted in terms of retrogressive (Brothers 1954; Borg 1956) or progressive (Ernst et al. 1970, p. 145) metamorphism. Calcic and alkali amphibole pairs in apparent equilibrium have been described independantly from four locations, (i) Ward Creek, Cazedero, California (Lee et al. 1966; Himmelberg & Papike 1969; Klein 1969), (ii) Tiburon Peninsula, California (Klein 1969; Ernst et al. 1970), (iii) Sanbagawa Metamorphic belt of Shikoku, Japan (Klein 1969; Ernst et al. 1970) and (iv) Knockmoral, Ayrshire (Bloxam & Allen 1960; Klein 1969). In addition, Klein and Himmelberg & Papike have separately reported occurrences from the Urals and New Caledonia respectively. Tie lines between apparently stably coexisting pairs are illustrated in plots of Al^{y} versus Na^{x} and Al^{z} versus Na^{x} in Figs 7.30 - 7.33.

With the exception of the pairs from the Sanbagawa Belt (Fig 7.32) the separation of the basic atomic formulae corresponds closely to the limits of those regions of A.C.S. in which basic atomic formulae are uncommon (cf Figs 7.1, 7.2, 7.4, 7.5, 7.25, 7.26 with Figs 7.30 - 7.33). This does not prove the existence of a solvus but is consistent with such an interpretation.

The tie lines offer no evidence for the extension of a solvus

Fig. 7.30 Apparently co-existing amphibole pairs from Ward Creek, Cazedero, California.

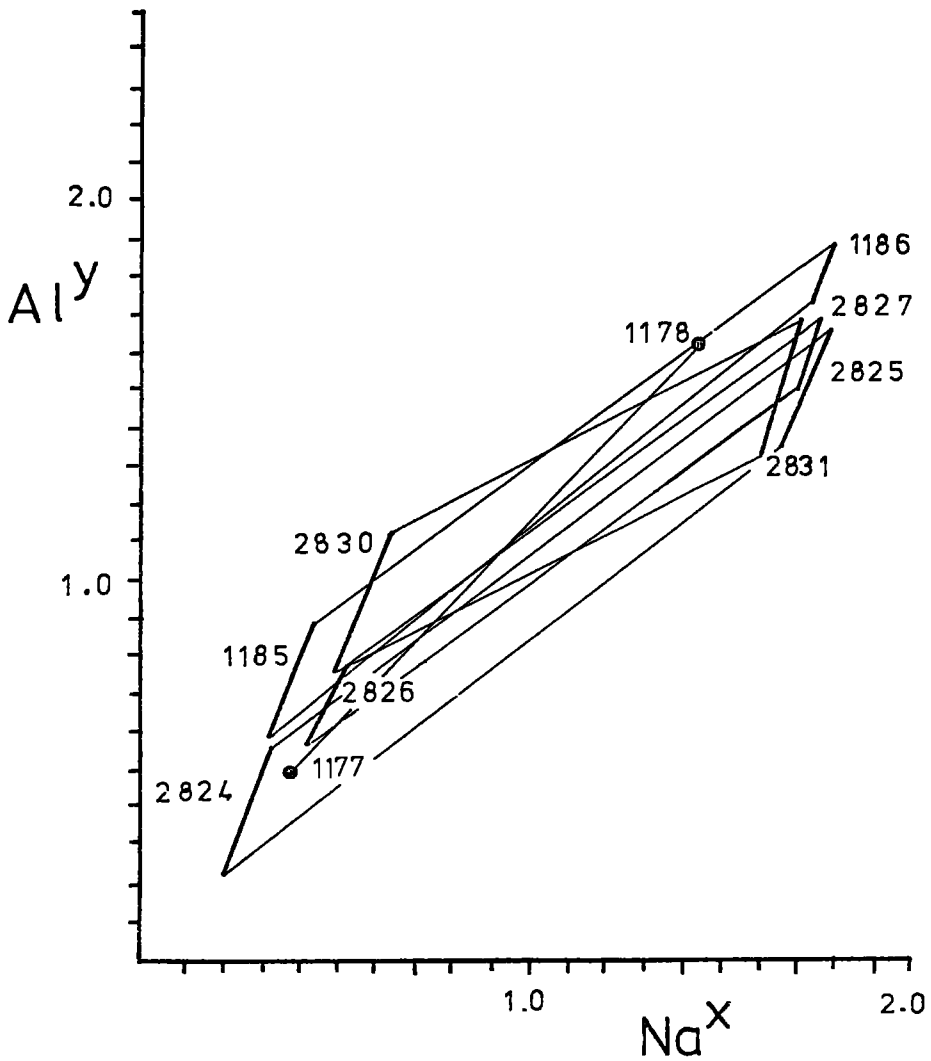
1177 - 1178 Lee et al. (1966) wet chemical analysis from metabasic block (two amphibole, muscovite, epidote, garnet, sphene, apatite, rutile), spec. no. 50-CZ-60. Klein (1969) and Himmelberg & Papike (1969) considered the purity of the analysed material was not very high.

2826 - 2827 Himmelberg & Papike (1969), replicate electron microprobe analysis of 1177- 1178.

2824 - 2825 Himmelberg & Papike (1969), electron microprobe analysis of metacarbonate (aragonite, garnet, two amphibole, stilpnomelane), spec. no. 201 - RGC - 59L.

2830 - 2831 Himmelberg & Papike (1969), electron microprobe analysis of metabasic block (two amphibole, omphacite, muscovite, epidote, garnet, sphene, apatite, rutile), spec. no. 29B-CZ-60.

1185 - 1186 Klein (1969), electron microprobe analysis from (omphacite, two amphibole, lawsonite, chlorite, pumpellyite, muscovite, sphene, pyrite), assemblage spec. no. 4-4.


2.0
1.0
Al y
1.0
2.0
Na x
1186
2827
2825
2831
1178
2830
1185
2826
1177
2824

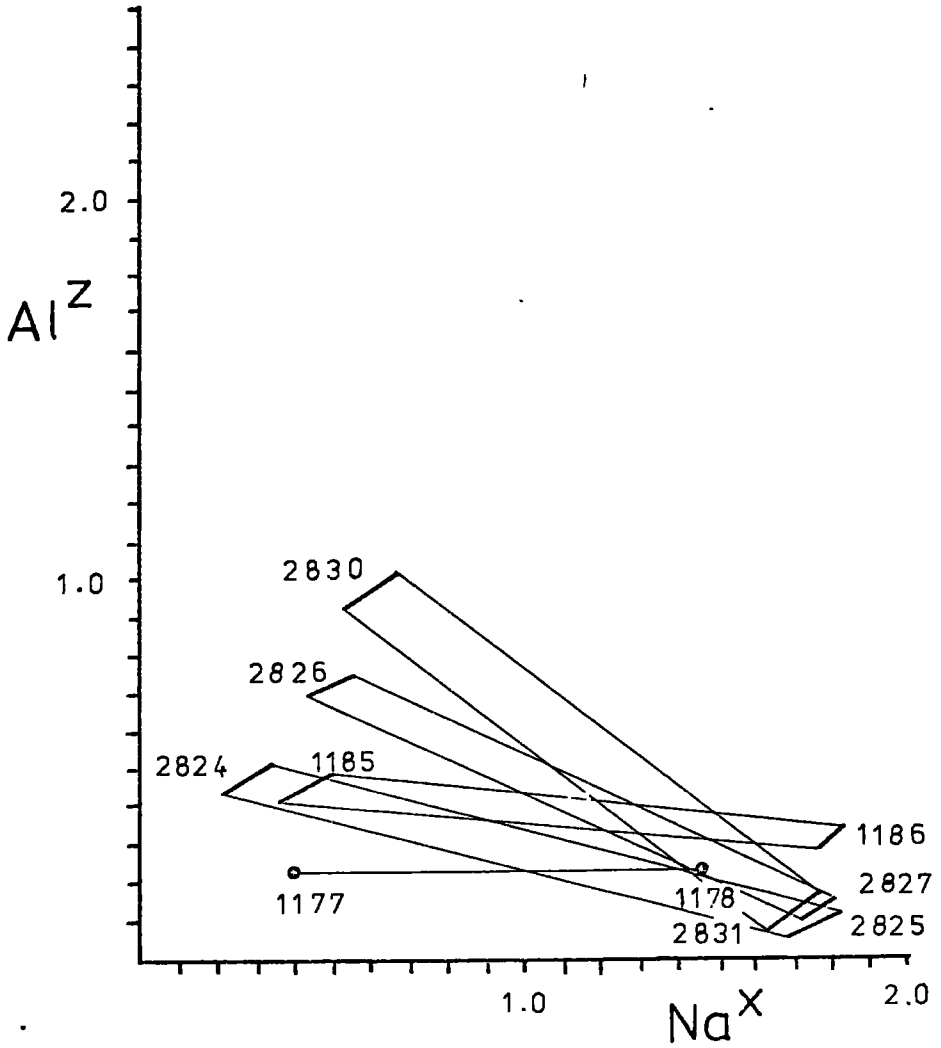

2.0
1.0
Al z
1.0
2.0
Na x
2830
2826
2824
1185
1186
2827
1178
2825
1177
2831

Fig. 7.31 Apparently co-existing amphibole pairs from the Tiburon Peninsula, California.

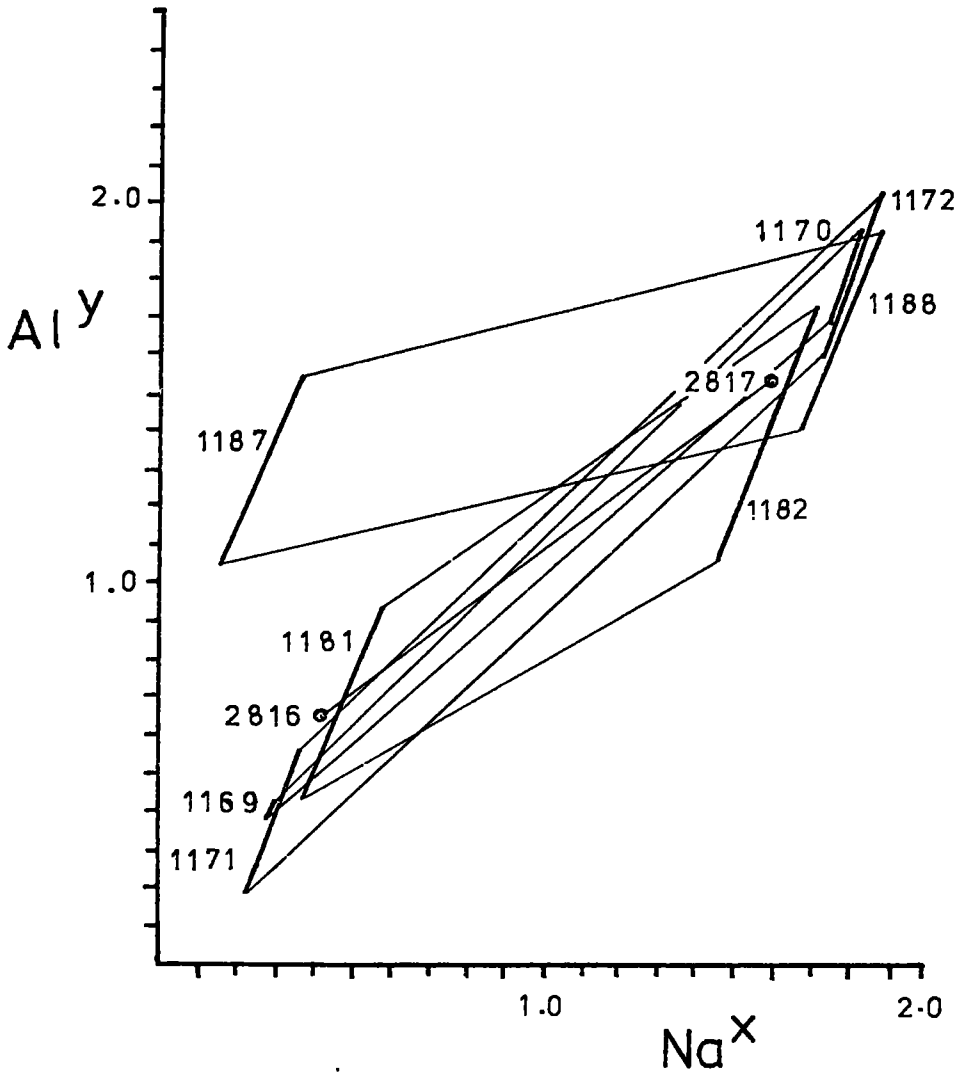
1169 - 1170 Klein (1969), electron microprobe analysis from a 'loose block' (epidote, two amphibole, lawsonite, sphene, chlorite, white mica,) spec. no. 3-1.

1171 - 1172 Klein (1969), electron microprobe analysis from a 'loose block' (epidote, garnet, two amphibole, omphacite, chlorite, mica, sphene, rutile, apatite, pumpellyite), spec. no. 3-2.

1181 - 1182 Klein (1969), electron microrprobe analysis from 'loose block' (garnet, two amphibole, sphene, rutile chlorite), spec. no. 4-2.

1187 - 1188 Klein (1969), electron microrprobe analysis from a 'loose block' (garnet, two amphibole, epidote, omphacite, chlorite, pumpellyite, rutile, sphene, apatite), spec. no. 4-5.

2816 - 2817 Ernst et al. (1970), wet chemical analysis from metabasalt 'loose block' (two amphibole, aragonite, white mica, chlorite, sphene), spec. no. GRS.


2.0
1.0
Al y
1.0
2.0
Na x
1172
1170
1188
2817
1187
1182
1181
2816
1169
1171

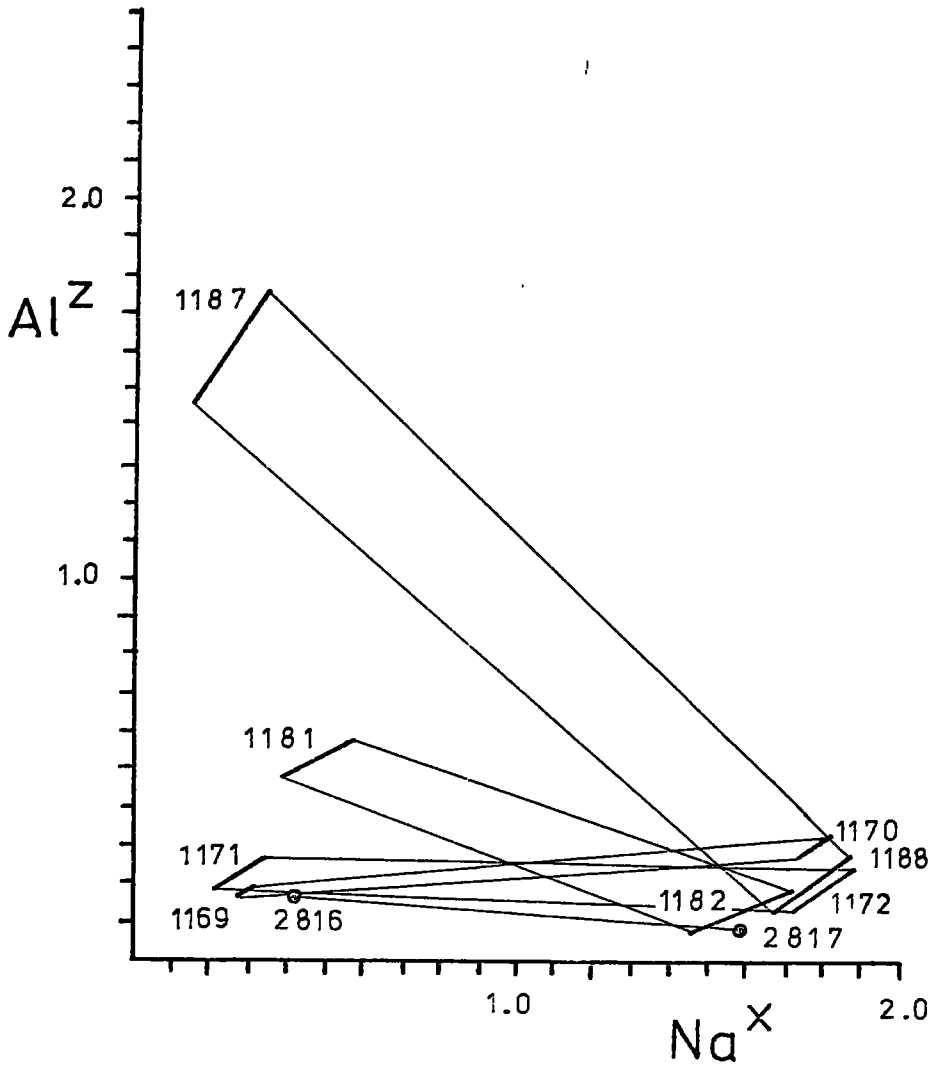
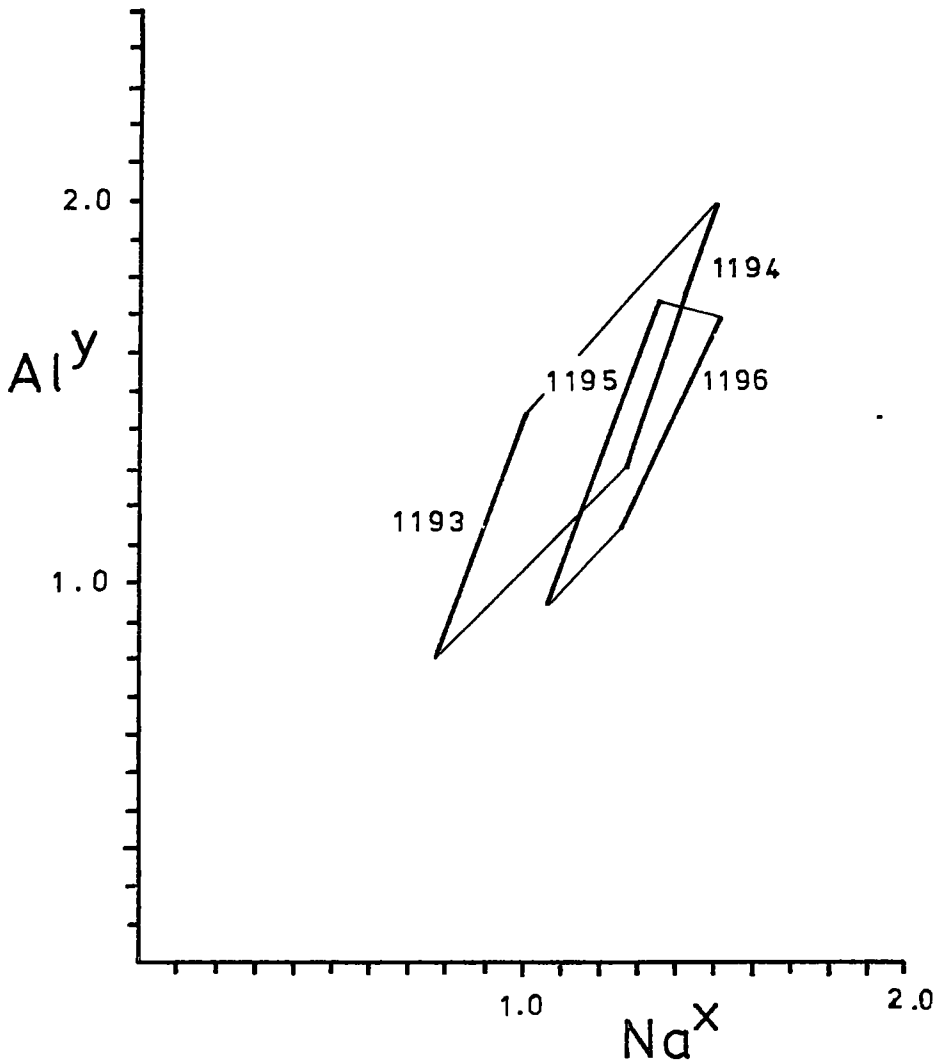

2.0
1.0
Al z
1.0
2.0
Na x
1187
1181
1170
1171
1188
1182
1172
1169
2816
2817

Fig. 7.32. Apparently co-existing pairs from the Sanbagawa Metamorphic Belt, Shikoku, Japan.

1193 - 1194 Klein (1969), electron microprobe analysis from (two amphibole, piedmontite, epidote, quartz, muscovite, garnet, chlorite) schist, spec. no. 5-2.

1195 - 1196 Klein (1969), electron microprobe analysis from (two amphibole, garnet, muscovite, quartz, apatite, haematite) schist, spec. no. 5-3.

Additional electron microrprobe analyses of pairs have been given by Ernst et al. (1970), 2818 - 2819 (S77B), 2820 - 2821, (S30G), 2822 - 2823 (S75B) and by Klein (1969), 1183 - 1184 (4-3), 1197 - 1198 (5-4) however in none of these is it explicitly stated that discrete grains are seen in contact.


2.0
1.0
Al^y
1193
1194
1195
1196
1.0
2.0
Na^x

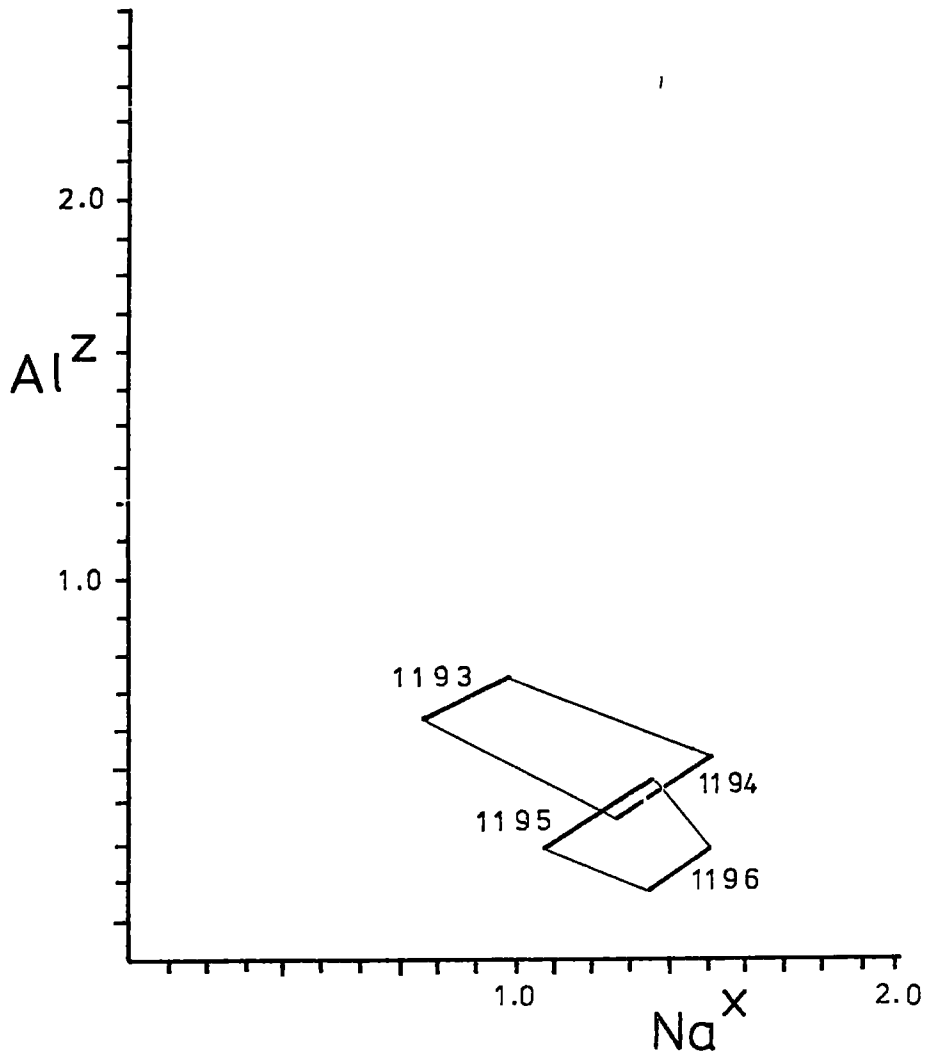

2.0
1.0
Al^z
1193
1194
1195
1196
1.0
2.0
Na^x

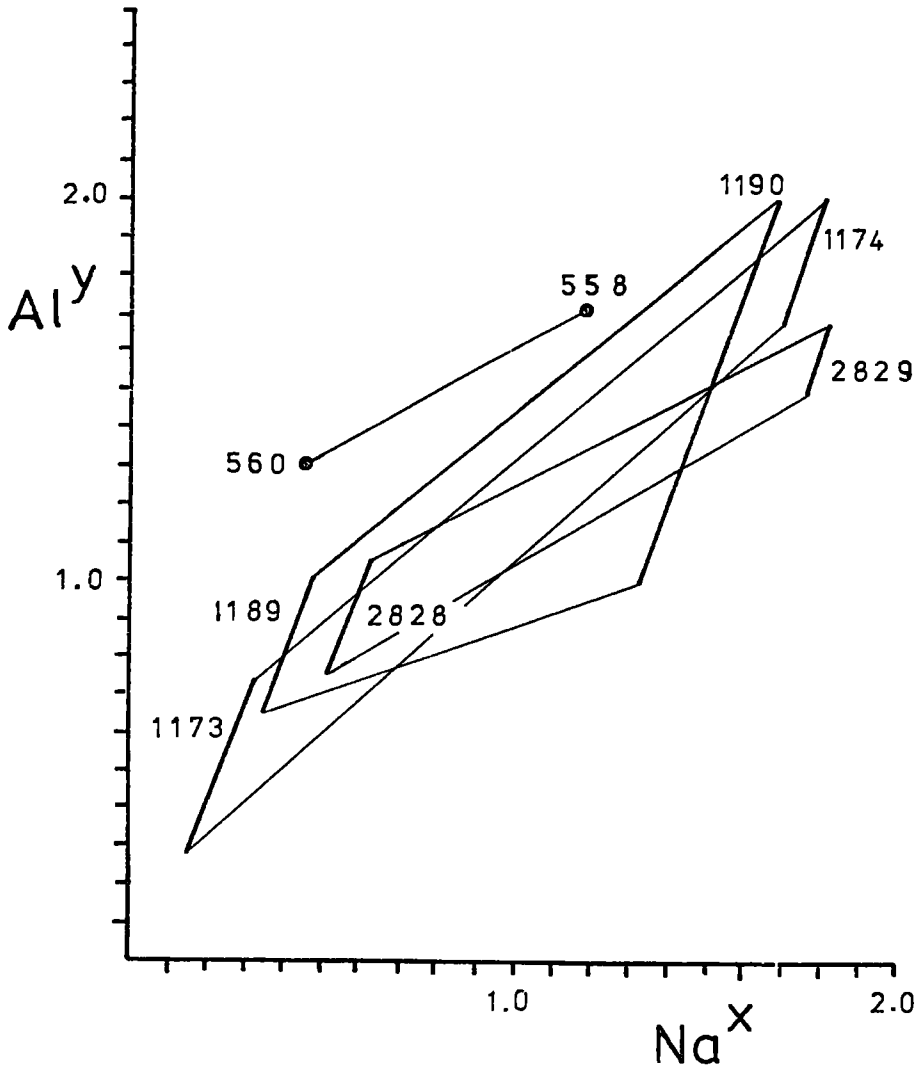
Fig. 7.33. Apparently co-existing amphibole pairs from various localities.

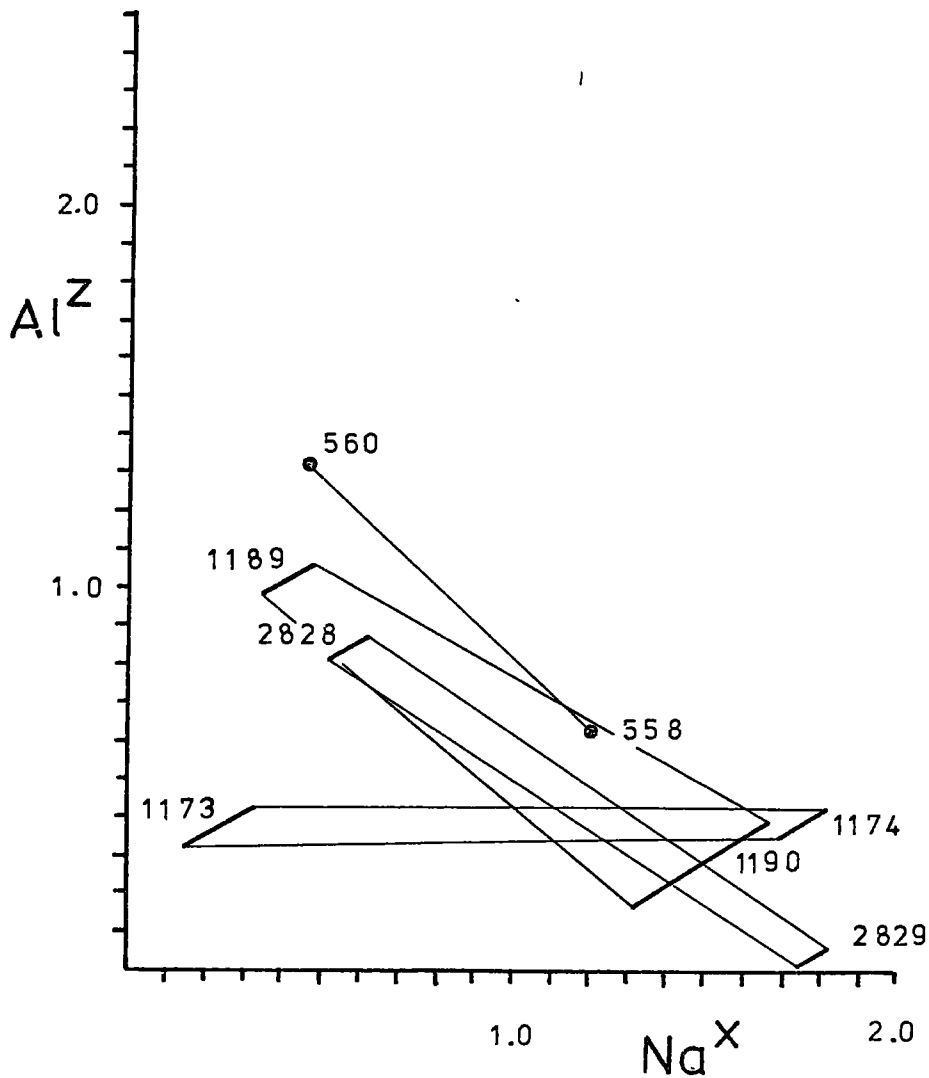
558 - 560 Bloxam & Allen (1960), wet chemical analyses from crossite amphibolite (epidote, two amphibole, sphene, albite, apatite, garnet), Knockmoral, Ayrshire, Bloxam pers. comm. in Klein (1969) suggested that there may be epidote impurity in 558.

1189 - 1190 Klein (1969), replicate electron microprobe analyses of 558 - 560.

2828 - 2829 Himmelberg & Papike (1969), electron microprobe analyses from metachert (quartz, garnet, two amphibole, epidote, haematite), New Caledonia, spec. no. 40-C.

1173 - 1174 Klein (1969), electron microrprobe analyses from (garnet, omphacite, two amphibole, quartz, mica, rutile, sphene, apatite, zircon), assemblage Southern Urals, spec. no. 3-3.


2.0
1.0
Al^y
Na^x
1.0
2.0
1190
1174
558
2829
560
1189
2828
1173


2.0
1.0
Al^z
Na^x
1.0
2.0
560
1189
2828
558
1173
1174
1190
2829

towards richterite.

Apart from the variation in Na^X and Al^Y which can be attributed to the coupled substitutions $CaMg^Y = Na^X Al^Y$ (Tr - G), and $Al^Y = Na^A Mg^Y$ (G - Ec) the basic atomic formulae of the alkali amphiboles are consistent in having Al^Z and Na^A less than 0.5. All have G as the dominant component of the basic atomic formulae. The calcic amphiboles are more variable especially with respect to Al^Z which ranges between 0.10 and 1.74. The A-site occupancy is also variable ranging between 0.04 - 0.76. These typically have Tr as the dominant component of the basic atomic formulae, although 2830 and 1189 pass into Pa s.d. at higher reduced iron ratios and 1187 is in Pa s.d. at all reduced iron ratios. The pairs from the Sanbagawa Metamorphic Belt are different with 1194, 1195, 1196 in G s.d. and 1193 in R s.d.

Parageneses in which these amphibole pairs occur are varied but as the whole rock chemistry and garnet compositions of Klein's (1969) analyses are not given it is difficult to assign them to specific metamorphic facies. However the following very tentative facies assignments have been made. 1193 - 1194, 1195 - 1196, 558 - 560 resemble parageneses of the greenschist facies with the addition of a soda calcic or alkali amphibole, 2824 - 2825, 1185 - 1186, 1169 - 1170, 2816 - 2817 resemble the glaucophane lawsonite schist facies of Turner (1968) or the low-temperature blueschists of Taylor & Coleman (1969), with the addition of a calcic amphibole, and 1177 - 1178, 2830 - 2831, 1171 - 1172, 1181 - 1182, 1187 - 1188, 2828 - 2829, 1173 - 1174 resemble the high-temperature blueschists of Taylor & Coleman (1969) with the omphacite bearing assemblages showing affinities to eclogites. Thus these two amphibole assemblages have apparently formed under conditions intermediate between the greenschist and glaucophane lawsonite schist facies or in the high-temperature blueschists.

If a solvus does exist then the low Al^z soda calcic amphiboles must be either hypersolvus, metastable, inhomogeneous, erroneous, or alternatively indicate that the solvus is restricted spatially in amphibole compositional space. In this connection all the low Al^z soda calcic amphiboles with balanced basic atomic formulae and either H_2O+, F or Cl determined have been plotted on Fig. 7.34 with all the coexisting pairs for comparison.

The occurrence and composition of the low Al^z soda calcic amphiboles illustrated in Figs 7.1 - 7.28 can be divided into two broad categories. Firstly, those from high temperature igneous or hydrothermal host rocks often associated with calcite or manganese mineralisation, for details see Fig. 7.34. These all have $Na^A > 0.2$, $Al^y < 1.08$ (except for 682 with Na^A 0.04, Al^y 1.49) and $Al^z < 0.77$. Apart from one amphibole each with Tr, G and Ec as the dominant component all the others are in the field or R sensu dominante. The remaining low Al^z soda calcic amphiboles in the amphibole data file in this category (1) have similar Na^A, Al^y and Al^z.

These soda calcic amphiboles may be considered as hypersolvus (Ernst 1968). Alternatively the distribution of these amphiboles on the low Al^y (richterite) side of the compositional break indicated by the amphibole pairs (Fig. 7.34) may indicate that the solvus, if any, does not extend tc richterite. This would also explain why miscibility relations have not been detected in the synthesis of richterite by Phillips & Rowbotham (1968), Huebner & Papike (1970), Forbes (1971), Charles (1972).

The second smaller category of low Al^z soda calcic amphiboles

- - - - - -

(1) 365 - 368 Carmichael (1967a); 2452, 2453, 2463, 2466 Kovalenko (1968); 1574, Nash,Carmichael & Johnson (1969); 1578, 1579 Nicholls &

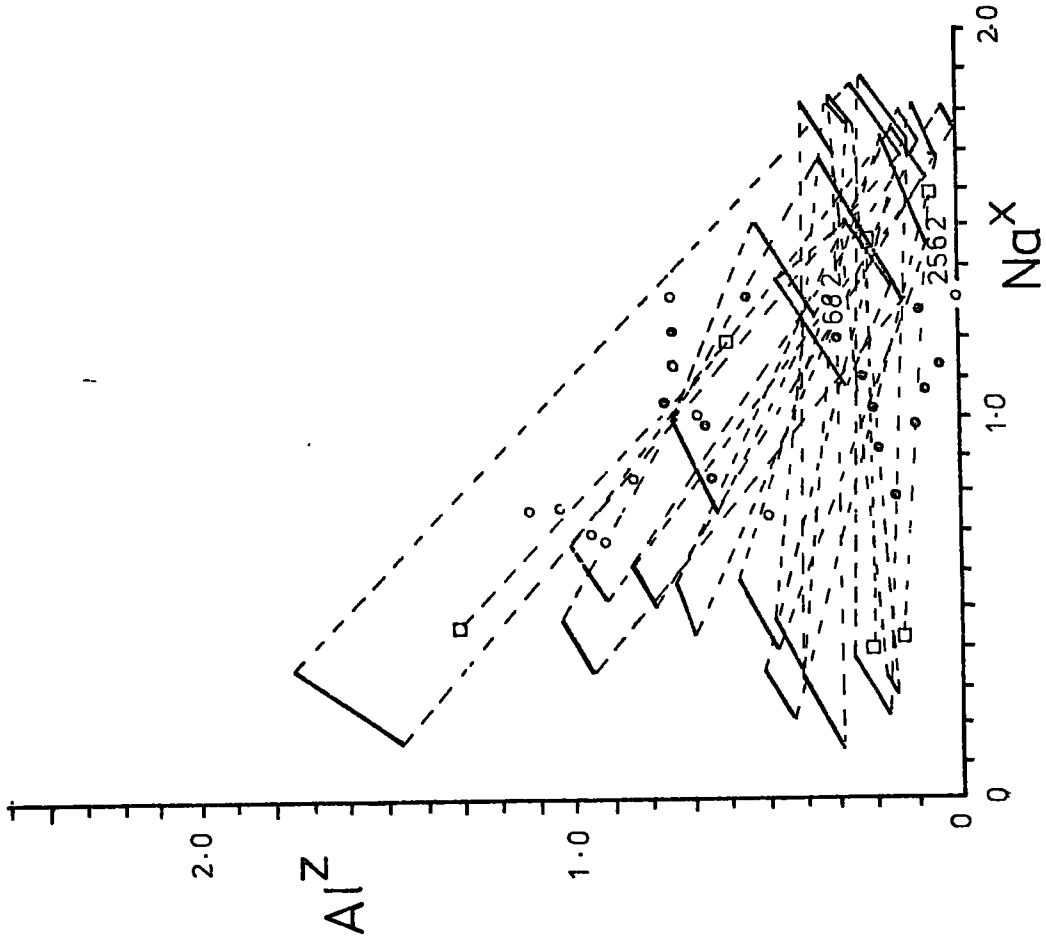
Fig. 7.34. Composite plot of apparently co-existing amphibole pairs and low Al^Z soda calcic amphiboles. The source and host rocks of the soda calcic amphiboles are as follows:-

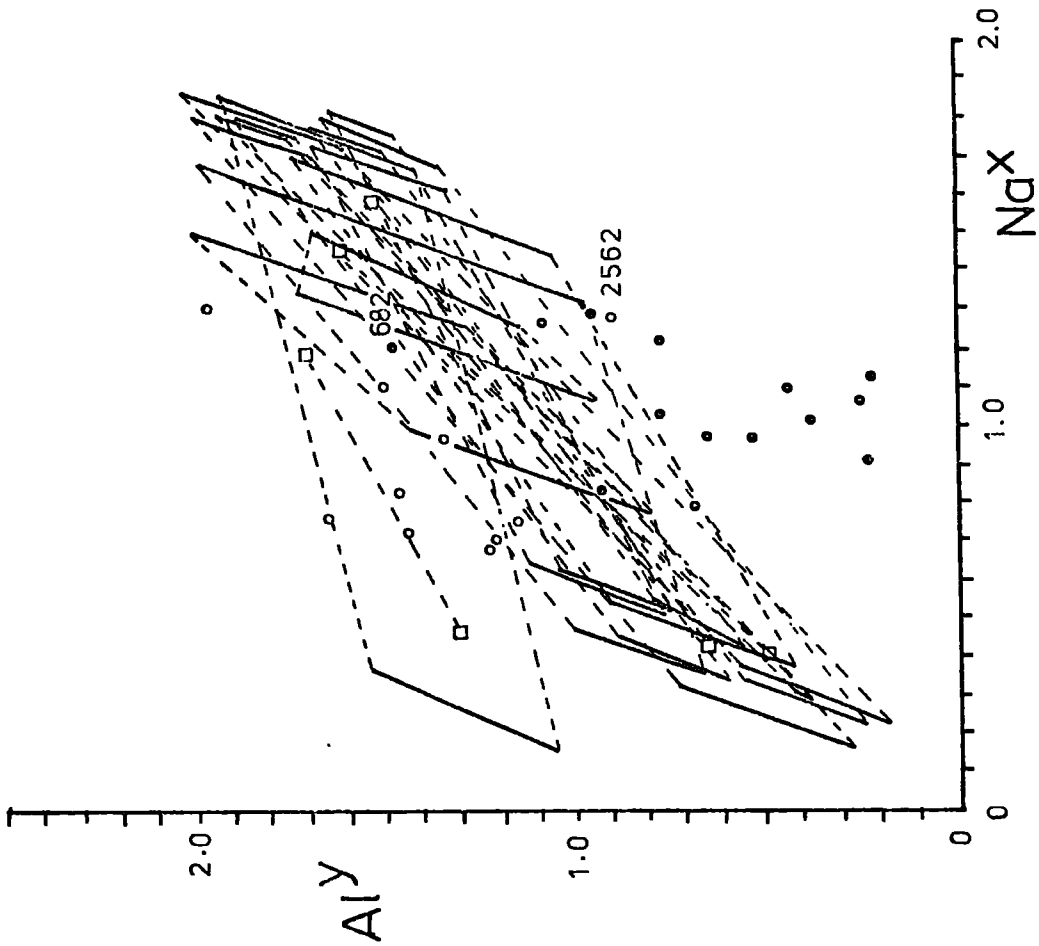
Igneous and hydrothermal host rocks ●

hydrothermal veins, 682 (Foshag 1936), 1311, 1313, 2832 (Larsen 1942); manganiferous skarns, 1833 (Rondolino 1936), 2810 (Sundius 1946), 1213 (Klein & Ito 1968); syenite, 592 (Erdsmannsdorffer 1929); carbonatite, 2159 (Sutherland 1969); fenite, 1739 (Perchuk et al. 1967); altered uncomphagrite 1319, 1320, 1321 (Larsen 1942); veinlets in serpentinite (Laudermik & Woodfor 1930); meteorite 2788 (Olsen 1967).

Metamorphic host rocks o

eclogites, 107 (omph., gar., amph, rutile, musc.), (Banno 1964), 385 (omph., amph., gar., epidote, quartz, chlorite, musc.) (Coleman et al. 1965), 190 (omph., gar., amph., rutile, apatite, quartz) (Binns 1967), 2812 (gar., omph., amph., rutile) (Ernst et al. 1970); metabasalt, 2203 (epidote, amph., albite, chlorite, musc.) (Iwasaki 1963), 97 (sphene, albite, epidote, haematite, chlorite, quartz, amph.) (Banno 1964), 598 (amph., epidote, chlorite, mica, quartz, sphene, albite, calcite), 599 (amph., epidote, mica, garnet, sphene, albite, quartz, chlorite) (Ernst 1964); ironstone, 2562 (specularite, magnesio riebeckite, cummingtonite, rhodonite) (Klein 1966).


2.0
1.0
0
Al^Z
0
1.0
2.0
Na^X
682
2562


2.0
1.0
Al^y
0
1.0
2.0
Na^X
682
2562

Carmichael (1969); 2564 - 2566, 2570, 2573, 2576, 2579 Woolley et al. (1972); 2840 - 2842 Erlank & Finger (1970); 2418 Frisch (1970).

- - - - - -

are from metamorphic host rocks and have basic atomic formulae with $Al^y > 1.17$, Al^z 0.5 - 1.12 (except 2562 with Al^y 0.90, Al^z 0.00 which plots with the first category) and $Na^A < 0.42$, see Fig. 7.34 for details. As might be expected for amphiboles close to the centre of amphibole compositional space the dominant component of the basic atomic formulae is varied and includes Tr, Ts, Su, G, but not R s.d. There are four other amphiboles in the amphibole data file which belong to this category. One of these 2561 a 'riebeckite - tremolite' from an amphibolite facies metamorphosed ironstone (Klein 1969) plots with analyses of the former category. The remaining three are electron microprobe analyses from metabasalts in the Sanbagawa Belt of Shikoku, 1197, 1198 (Klein 1969) and 2822 (Ernst et al. 1970). 1197, 1198 represent zones in amphibole from a quartz, albite, chlorite, amphibole stilpnomelane, mica, piedmontite, garnet, sphene assemblage which yield basic atomic formulae of Na^A 0.30 - 0.53, Al^y 0.79 - 1.23, Al^z 0.66 - 0.78 and Na^A 0.03 - 0.45, Al^y 0.76 - 1.36, Al^z 0.45 - 0.57 respectively while 2822 which is mantled by non-equilibrium calcic amphibole gave the following basic atomic formulae Na^A 0.07 - 0.36, Al^y 1.29 - 1.98, Al^z 0.34 - 0.48.

There are thus twelve amphiboles in this second category which can be considered as intermediate between at least some of the apparently stably coexisting pairs (97, 107, 190, 385, 598, 599, 991, 1197, 1198, 2203, 2812, 2822). The combination of evidence from the distribution of basic atomic formulae in A.C.S. and the adjacent portion of E.A.C.S., the close correspondence of the compositional gap between amphiboles in apparent equilibrium with the observed distribution, and the presence of only twelve analyses out of 2560

in the amphibole data file which are intermediate is consistent with the existence of a solvus although this probably does not extend to richterite.

Interpretation of the twelve intermediate analyses is difficult. 2202 (Van der Plas & Hugi 1961; Klein 1969) is an analysis of composite material. Three of the amphiboles from eclogites (107 Banno 1964; 190 Binns 1967; 2812 Ernst et al. 1970) are associated with rocks of the albite epidote amphibolite facies and might conceivably be hypersolvus. The fourth eclogite 385 Coleman et al. 1965) was not found in situ. Seven others (97 Banno 1964; 598, 599 Ernst 1964; 991 Iwasaki 1963; 1197, 1198 Klein 1969; 2822 Ernst et al. 1970), are from the Sanbagawa belt of Shikoku. It is tempting to correlate these soda calcic amphiboles with the narrow compositional gap illustrated in Fig. 7.32 as indicating the reduction or elimination of a solvus under the conditions appropriate to the Sanbagawa Belt. However the non-equilibrium nature of 1197, 1198, 2822 and the reported 3 to 4 per cent epidote impurity in the analysed material of 589, 590 complicates the interpretation of these analyses. It is suggested therefore that a solvus does separate the calcic and alkali amphiboles under at least some metamorphic conditions but that this solvus probably does not extend to richterite.

8. GENERAL FEATURES OF THE BASIC ATOMIC FORMULAE OF AMPHIBOLES FROM THE MAJOR IGNEOUS AND METAMORPHIC PARAGENESES.

In this Chapter the general features and distribution of basic atomic formulae from ultramafic - ultrabasic, basic, intermediate, acid, basic alkali and alkali igneous host rocks and calcareous, ferruginous, serpentinite, eclogite and the remaining metamorphic host rocks will be described. It must be emphasised that allocation of an amphibole to one of these categories is based on the original author's name for the host rock type (Chapters 4, 7). It has only been possible to verify this and to separate amphiboles which are secondary or in non-equilibrium in a limited number of instances of special significance. Unfortunately amphiboles from metabasics and metapelites from contact and greenschist, albite epidote amphibolite, amphibolite, granulite, glaucophane lawsonite schist and intermediate facies have not been distinguished. Ideally the writer would have liked to have separated amphiboles from each of the major facies but this proved inpractical. Statements of the metamorphic facies are not always given with analyses of amphiboles and it would have been a considerable task to determine the facies from stated mineral assemblages. The characteristic features of the basic atomic formulae of amphiboles from each of the above parageneses are discussed below as follows, ultramafic - ultrabasic Section 8.1.1, basic Section 8.1.2, intermediate Section 8.1.3, acid Section 8.1.4, basic alkali Section 8.1.5 and alkali Section 8.1.6, igneous parageneses and calcareous Section 8.2.1, ferruginous Section 8.2.2, serpentinite Section 8.2.3, eclogite Section 8.2.4 and the remaining metamorphic parageneses Section 8.2.5. The general features of amphiboles from particular host rocks and the relation between host rock type and amphibole composition is discussed in Section 8.3.

Table 8.1 summarises the nomenclature and extent of Mg^{2+} - Fe^{2+}

Table 8.1. Nomenclature and $Mg^{2+} - Fe^{2+}$, $Al^{vi} - Fe^{3+}$ substitution in amphiboles from various igneous and metamorphic host rock categories.

		Sensu dominante												
		Tr	Ed	Pa	Ts	Su	R	G	Ec	M	Ks	No	UNNAMED	FeMgMn
Mg^{2+} Al^{vi}	Ultramafic - ultrabasic	3	-	22	4	4	-	-	-	-	1	-	-	-
Mg^{2+} Fe^{3+}		1	1	15	-	7	2	-	-	-	2	1	-	-
Fe^{2+} Al^{vi}		-	-	-	-	-	-	-	-	-	-	-	-	-
Fe^{2+} Fe^{3+}		-	-	-	-	-	-	-	-	-	-	-	-	-
total		4	1	37	4	11	2	-	-	-	3	1	-	-
Mg^{2+} Al^{vi}	Basic	6	-	12	12	-	-	-	-	-	-	-	-	1
Mg^{2+} Fe^{3+}		3	-	8	5	3	-	-	-	-	3	-	-	-
Fe^{2+} Al^{vi}		-	-	-	1	1	-	-	-	-	-	-	-	-
Fe^{2+} Fe^{3+}		-	-	2	4	-	-	-	-	-	-	1	-	-
total		9	-	22	22	4	-	-	-	-	3	1	-	1
Mg^{2+} Al^{vi}	Intermediate	3	-	4	8	1	-	-	-	-	-	-	-	-
Mg^{2+} Fe^{3+}		26	-	17	15	2	-	-	-	-	-	-	-	-
Fe^{2+} Al^{vi}		1	-	1	-	-	-	-	-	-	-	-	-	-
Fe^{2+} Fe^{3+}		1	-	4	3	2	-	-	-	-	-	-	-	-
total		31	-	26	26	5	-	-	-	-	-	-	-	-
Mg^{2+} Al^{vi}	Acid	3	-	2	4	-	-	-	-	-	-	-	-	-
Mg^{2+} Fe^{3+}		18	-	6	18	-	-	2	-	-	-	-	-	1
Fe^{2+} Al^{vi}		-	-	2	1	-	-	-	-	-	-	-	-	1
Fe^{2+} Fe^{3+}		-	-	21	4	-	-	3	7	-	-	-	-	-
total		21	-	31	27	-	-	5	7	-	-	-	-	2

		Tr	Ed	Pa	Ts	Su	R	G	Ec	M	Ks	No	UNNAMED	FeMgMn
$g^{2+}Al^{vi}$	Basic alkali	-	-	-	1	1	-	1	-	-	3	-	-	-
$g^{2+}Fe^{3+}$		3	-	6	-	5	2	-	2	-	13	1	-	-
$e^{2+}Al^{vi}$		-	-	-	-	-	-	-	-	-	-	-	-	-
$e^{2+}Fe^{3+}$		-	-	-	-	-	-	-	-	-	-	-	-	-
total		3	-	6	1	6	2	1	2	-	16	1	-	-
$g^{2+}Al^{vi}$	Alkali	1	-	-	-	-	-	-	-	-	-	-	-	-
$g^{2+}Fe^{2+}$		3	-	2	-	-	3	2	9	-	-	-	-	-
$e^{2+}Al^{vi}$		-	-	3	-	-	-	-	1	-	-	1	-	-
$e^{2+}Fe^{3+}$		-	-	27	1	7	-	5	6	1	2	2	-	-
total		4	-	32	1	7	3	7	16	1	2	3	-	-
gneous total		72	1	154	81	33	7	13	25	1	24	6	-	3

Sensu Dominante

	Tr	Ed	Pa	Ts	Su	R	G	Ec	M	Ks	No	UNNAMED	FeMgMn
Calcareous metamorphic													
g^{2+},Al^{vi}	21	4	6	1	-	-	-	-	-	-	-	-	-
g^{2+},Fe^{3+}	7	2	4	-	-	1	2	3	-	-	-	-	-
e^{2+},Al^{vi}	1	-	6	-	-	-	-	-	-	-	-	-	-
e^{2+},Fe^{3+}	1	-	8	-	-	-	-	-	-	-	-	-	-
total	30	6	24	1	-	1	2	3	-	-	-	-	-
Ferruginous metamorphic													
g^{2+},Al^{vi}	7	-	-	-	-	-	-	-	-	-	-	-	3
g^{2+},Fe^{3+}	2	-	-	-	-	-	1	-	-	-	-	-	1
e^{2+},Al^{vi}	-	-	-	-	-	-	-	-	-	-	-	-	-
e^{2+},Fe^{3+}	1	-	-	-	-	-	3	-	-	-	1	-	10
total	10						4				1	-	14
Serpentinite													
g^{2+},Al^{vi}	3	-	1	-	-	1	-	-	-	-	-	-	1
g^{2+},Fe^{3+}	-	-	-	-	-	-	-	-	-	-	-	-	-
e^{2+},Al^{vi}	-	-	-	-	-	-	-	-	-	-	-	-	-
e^{2+},Fe^{3+}	-	-	-	-	-	-	-	-	-	-	-	-	-
total	3	-	1	-	-	1	-	-	-	-	-	-	1
Eclogite													
g^{2+},Al^{vi}	2	-	9	7	4	-	3	-	-	1	-	-	-
g^{2+},Fe^{3+}	1	-	1	2	-	-	-	-	-	-	-	-	-
e^{2+},Al^{vi}	-	-	-	1	-	-	-	-	-	-	-	-	-
e^{2+},Fe^{3+}	-	-	-	-	-	-	-	-	-	-	-	-	-
total	3	-	10	10	4	-	3	-	-	1	-	-	-
Remaining metamorphic													
g^{2+},Al^{vi}	46	7	78	105	-	-	21	-	-	-	6	2	30
g^{2+},Fe^{3+}	34	13	66	55	4	-	4	-	1	-	1	-	6
e^{2+},Al^{vi}	1	1	6	29	1	-	-	-	-	-	3	1	1
e^{2+},Fe^{3+}	1	1	20	7	4	-	4	-	1	-	1	-	-
total	82	22	170	196	9	-	29	-	2	-	11	3	37
tamorphic total	128	28	205	207	13	2	38	-	2	1	12	3	52

and $Al^{vi} - Fe^{3+}$ substitution in those amphiboles in the amphibole data file with either H_2O+, F or Cl determined and yielding balanced basic atomic formulae. Sensu dominante names for the calcic, soda calcic and alkali amphiboles, as defined in Chapter 7, were obtained with the aid of Table 5.1. Where it was not possible to obtain a sensu dominante name for a calcic, soda calcic or alkali amphibole the analysis has been entered under the column headed 'No'. Kaersutites as defined in Section 5.5.1, were separated and are shown as the column head 'Ks'.

8.1. Amphiboles from igneous host rocks.

From an inspection of Figs 7.1 - 7.28 and Table 8.1 it can be seen that the great majority of amphiboles from igneous host rocks are either calcic, soda calcic or alkali amphiboles. Only three analyses, two cummingtonites and one grunerite plot in the FeMgMn amphiboles. Since the remaining analyses have Mg^X less than 0.66 and are either calcic, soda calcic or alkali amphiboles it is possible to illustrate the variation in Al^z, Al^y, and Na^X in the basic atomic formulae in terms of two axis plots of Al^z versus Na^X and Al^z versus Al^y. This has been done for each of the six igneous host rock categories, Figs 8.1 - 8.6. The distributions differ from Figs 7.21, 7.22 in the inclusion of basic atomic formula with Mg^X up to 0.66.

Considering each of the categories in turn.

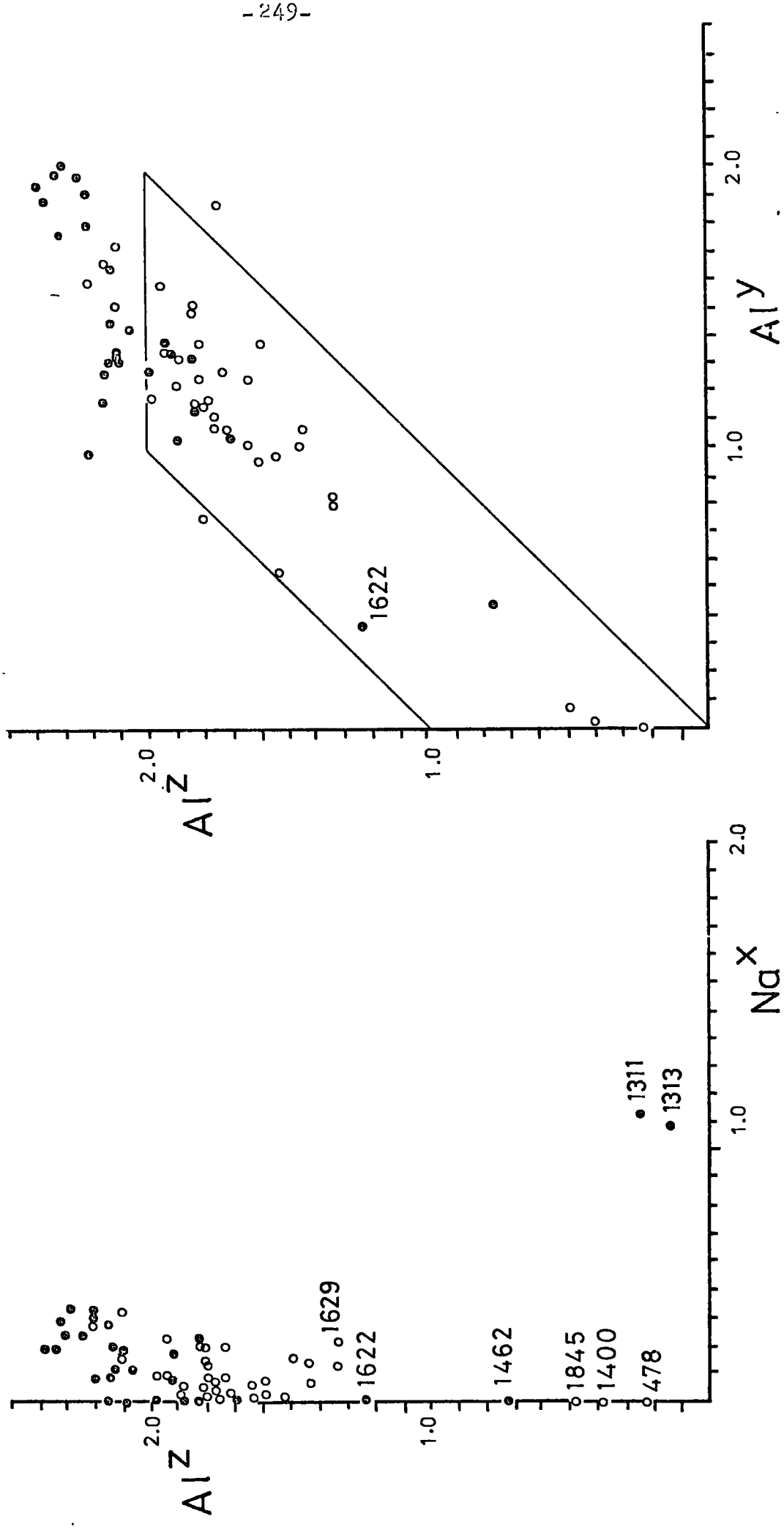
8.1.1. Ultramafic - ultrabasic. (Table 8.1, Fig. 8.1).

With two exceptions, 1311 and 1313, both in R s.d., which are replicate analyses of amphibole in a pyroxenite adjacent to a hydrothermal vein (Larsen 1938, 1942) all the remaining amphiboles from ultramafic - ultrabasic host rocks are calcic. Al^z and Al^y range between limits of 0.2 to 2.4, and 0.0 to 2.0 respectively. There are only seven analyses with Al^z less than 1.4 . In terms of

Figs. 8.1 - 8.6 Al^{Z} versus Na^{X} for calcic, soda calcic and alkali amphiboles and Al^{Z} versus Al^{Y} for calcic amphiboles from ultramafic - ultrabasic (8.1), basic (8.2), intermediate (8.3), acid (8.4), basic alkali (8.5), and alkali (8.6) igneous host rocks. Substitutions in the atomic formulae are indicated as follows:-

$Fe^{2+}/(Fe^{2+} + Mg^{2+})$	$Fe^{2+}/(Fe^{2+} + Al^{vi})$	Abbrev.	Symbol.
$\leqslant 0.5$	$\leqslant 0.5$	(Mg^{2+},Al^{vi})	○
$\leqslant 0.5$	> 0.5	(Mg^{2+},Fe^{2+})	◍
> 0.5	$\leqslant 0.5$	(Fe^{2+},Al^{vi})	△
> 0.5	> 0.5	(Fe^{2+},Fe^{3+})	▲

Fig. 8.1.


Al z
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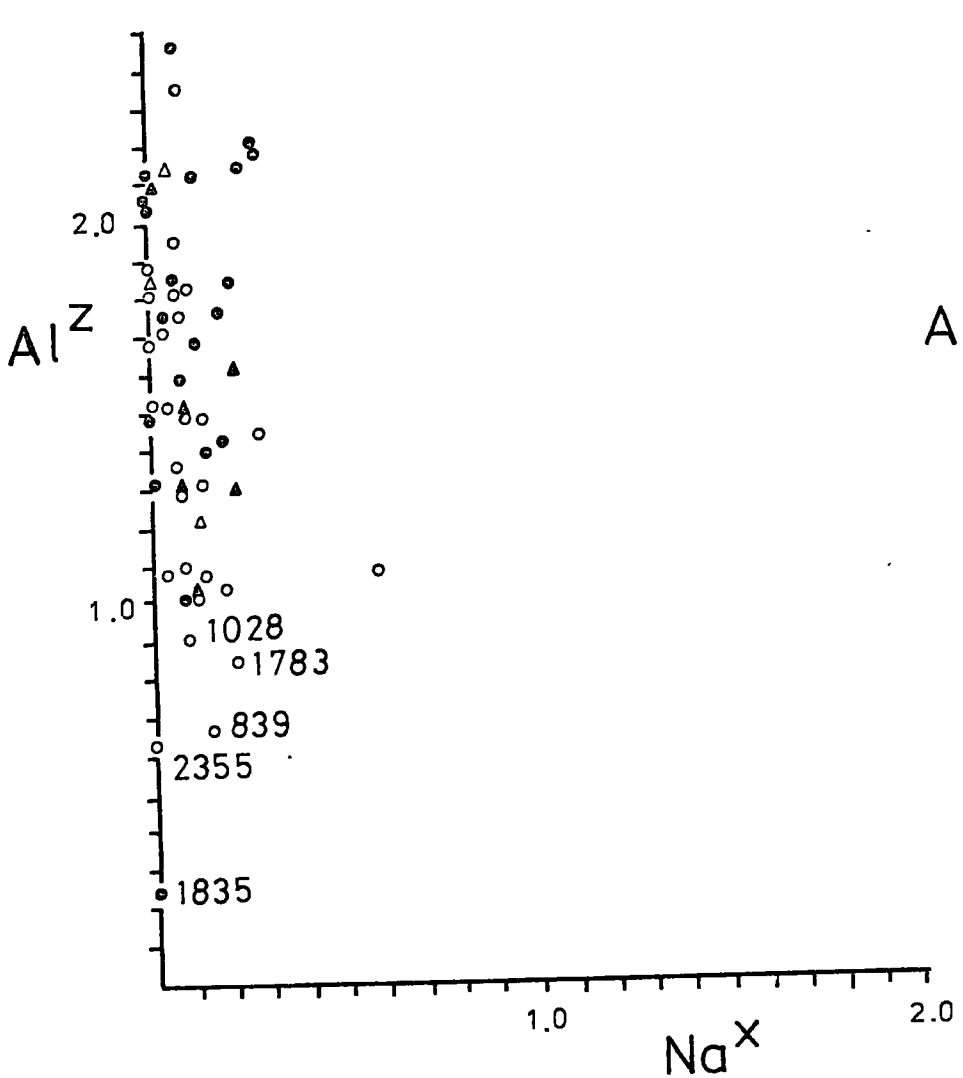
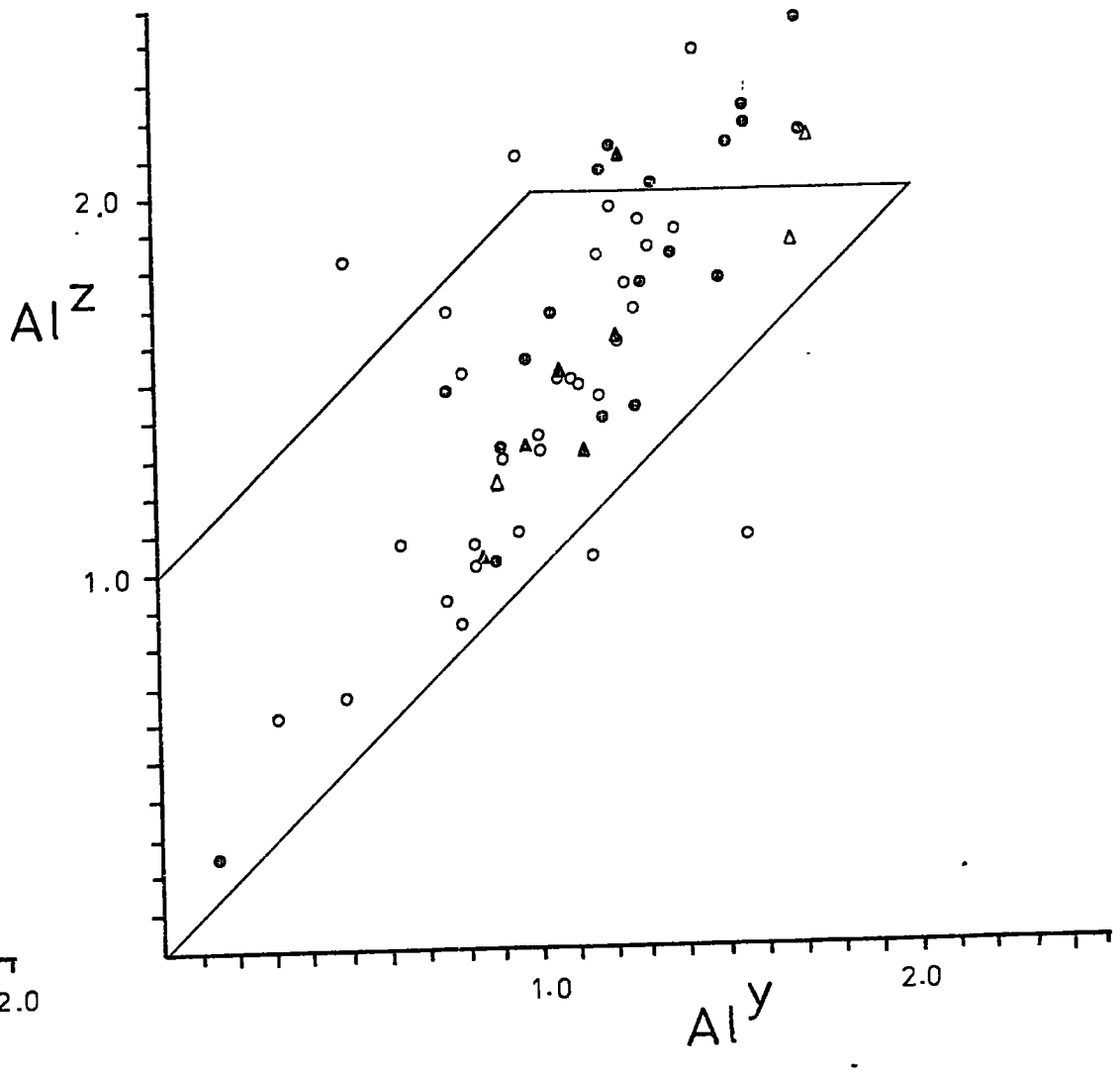
1.0
1622
Al y
2.0
1.0
Al z
2.0
1.0
1629
1622
1462
1845
1400
478
1311
1313
Na x
1.0
2.0

Fig. 8.2.





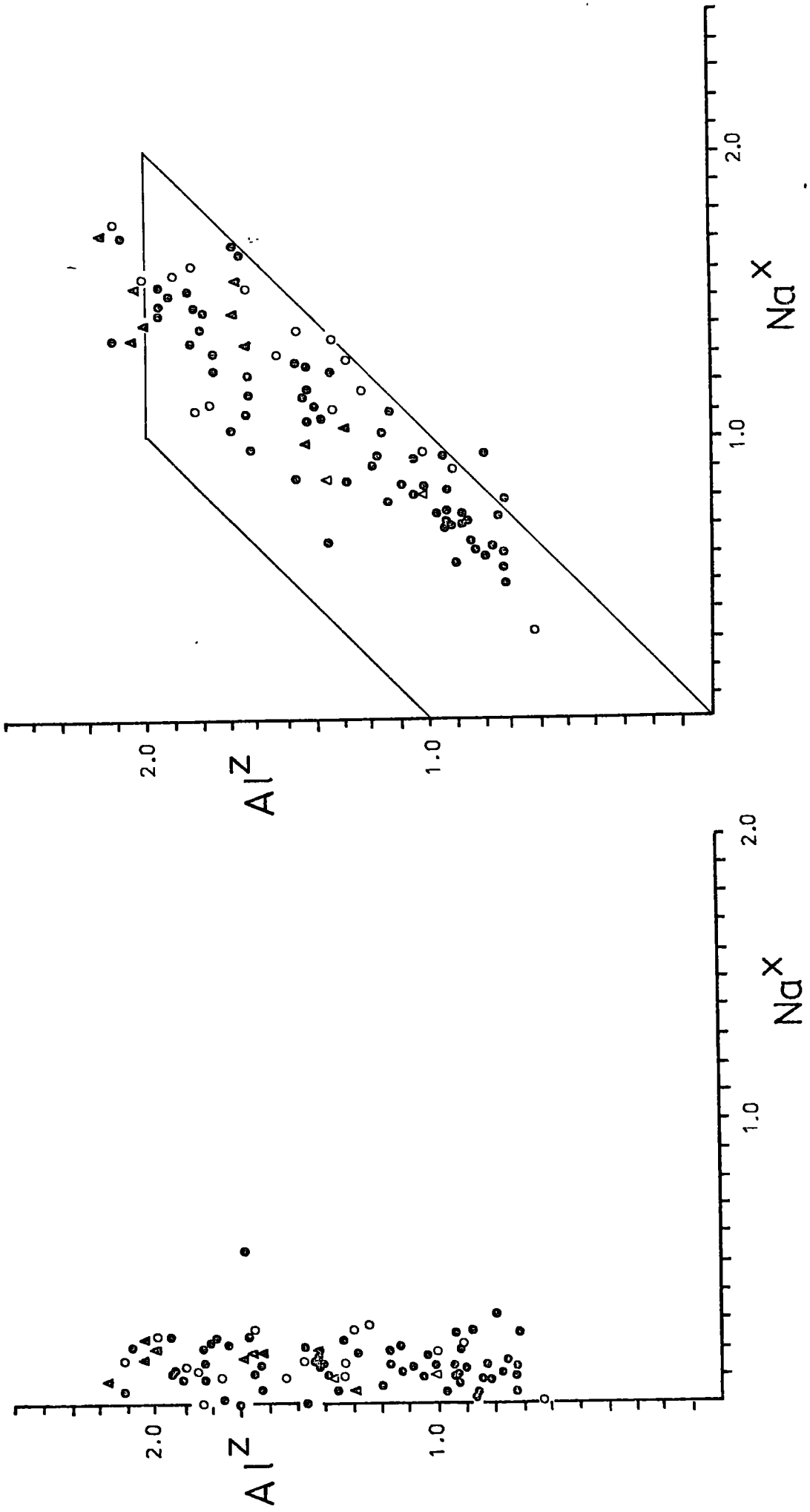


Fig. 8.3.

Fig. 8.4.

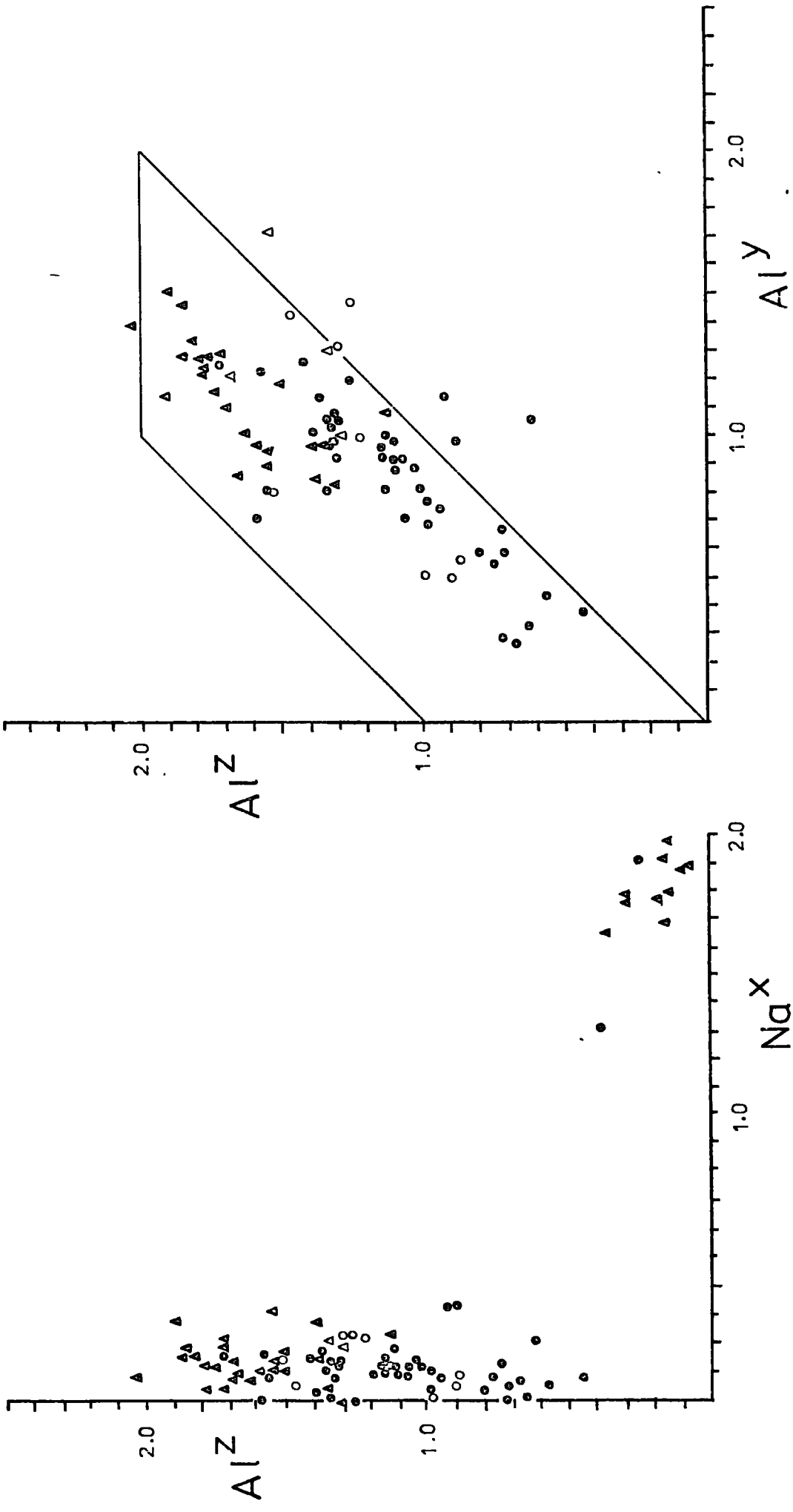


Fig. 8.5.

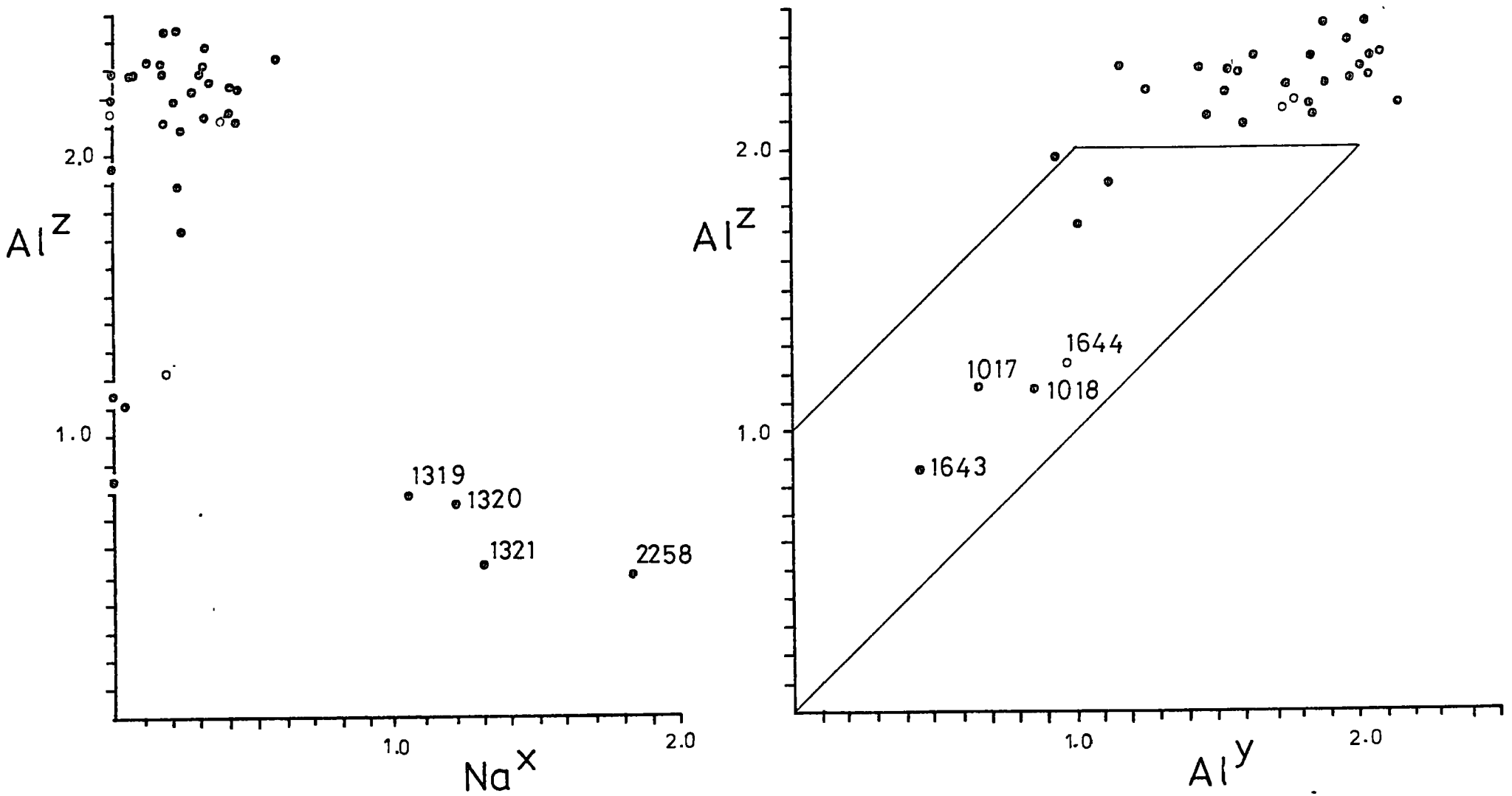
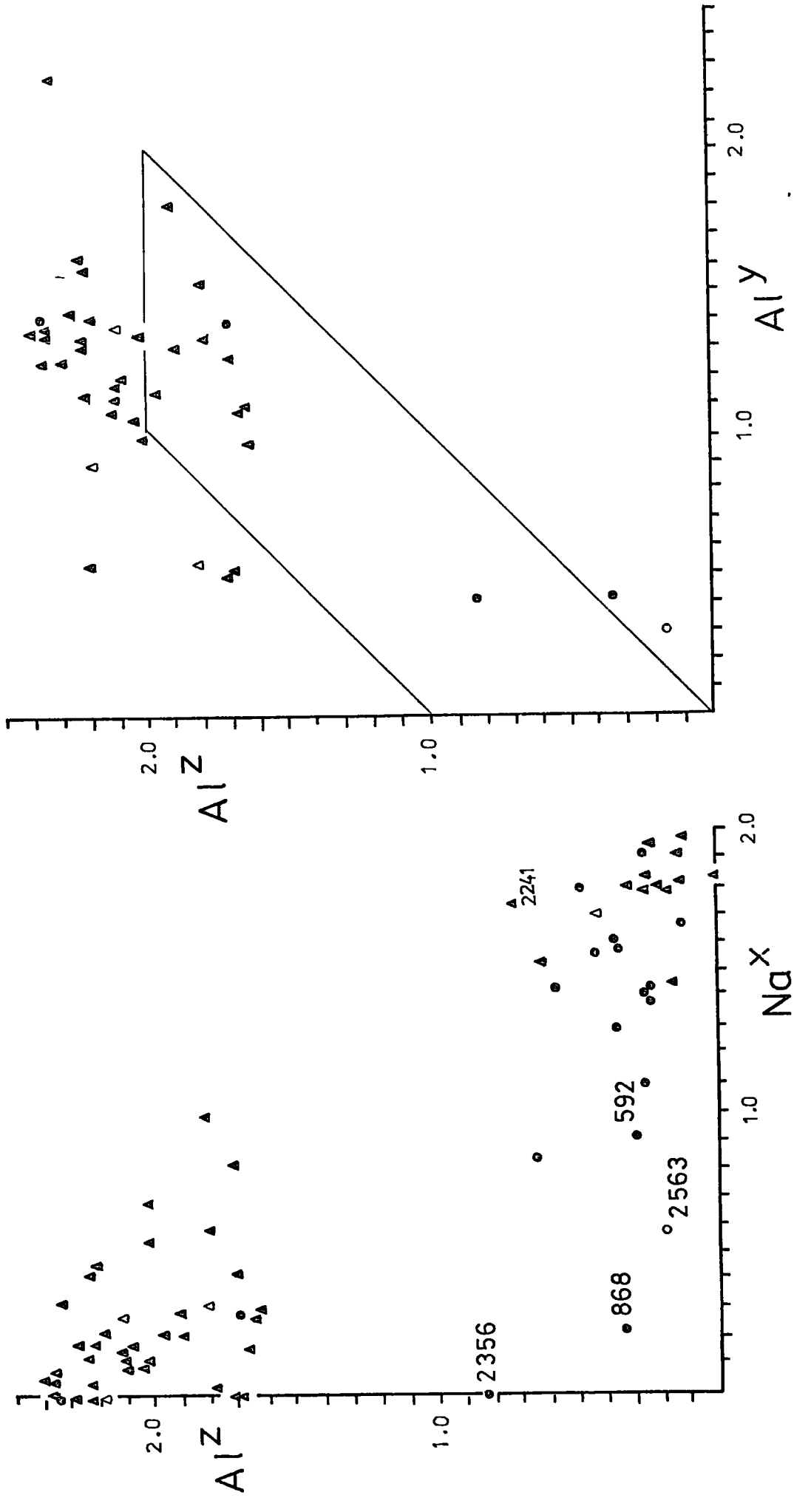

Al^z
2.0
1.0
1319
1320
1321
2258
1.0
2.0
Na^x
Al^z
2.0
1.0
1644
1017
1018
1643
1.0
2.0
Al^y

Fig. 8.6.



sensu dominante nomenclature, amphiboles from ultramafic - ultrabasic host rocks belong predominantly to Pa s.d. and less commonly to Su, Ts, and Tr s.d. In addition, there are three kaersutites and a single analysis, 1622 (Onuki 1963) in the field of Ed s.d. The four analyses from Tr s.d., 478 (Du Rietz 1935), 1400 (Lukac 1935), 1462 (Mikola & Sahama 1936), 1845 (Ross 1929) are all secondary after pyroxene or olivine. All basic atomic formulae are either (Mg^{2+}, Al^{vi}) or (Mg^{2+}, Fe^{3+}) substituted.

8.1.2. Basic. (Table 8.1. Fig. 8.2).

With the exception of one cummingtonite, 2838, (Savolahti 1966) all amphiboles from basic igneous host rocks are calcic. Al^{z} and Al^{y} range between 0.2 to 2.5 and 0.1 to 1.8 respectively. With five exceptions Al^{z} is in excess of 1.0. The analyses are equally distributed between the fields of Pa and Ts s.d. with less common Tr and Su s.d. There are also three kaersutites. The five analyses with Al^{z} less than 1.0, 839 (Henry), 1028 (Kanisawa 1964), 1783 (Ramachandra 1937), 1835 (Rose & Fromme 1932), 2355 (Yosyimura 1940) all in the field ot Tr s.d. are secondary. There are no analyses in Ed s.d. Basic atomic formulae are predominantly, but no exclusively, (Mg^{2+}, Al^{vi}) and (Mg^{2+}, Fe^{3+}) substituted.

8.1.3. Intermediate. (Table 8.1, Fig. 8.3).

All the amphiboles from intermediate igneous host rocks are calcic. Al^{z} and Al^{y} range between 0.6 to 2.2. and 0.3 to 1.7 respectively. The analyses are almost equally distributed between the fields of Tr, Pa and Ts s.d. with some in Su s.d. There are no kaersutites or analyses with Ed as the dominant component. Basic atomic formulae are predominantly (Mg^{2+}, Fe^{3+}) and less commonly (Mg^{2+}, Al^{vi}), (Fe^{2+}, Fe^{3+}) substituted. In contrast to the preceding categories Fe^{3+} excedes Al^{vi} in the majority of instances.

8.1.4. Acid. (Table 8.1. Fig. 8.4).

Apart from one cummingtonite, 302 (Buckley & Wilkins 1971) and one grunerite, 1014 (Bowen & Schairer 1935) all remaining amphiboles from acid igneous host rocks are either calcic, soda calcic or alkali. Taking the calcic amphiboles first, Al^z, Al^y, range between 0.4 to 2.1 and 0.2 to 1.7 respectively and the analyses are distributed between Pa, Ts and Tr s.d. There are no analyses in Ed or Su s.d. and no kaersutites. The basic atomic formulae are characteristically (Mg^{2+}, Fe^{3+}) or (Fe^{2+}, Fe^{3+}) substituted with (Fe^{2+}, Fe^{3+}) basic atomic formulae concentrated in Pa s.d.

The soda calcic and alkali amphiboles have $Al^z < 0.4$, Al^y 0.8 - 2.1 and belong to Ec and G s.d. The A site occupancy ranges from 0.11 to 1.16. With two exceptions all the basic atomic formulae are (Fe^{2+}, Fe^{3+}) substituted. The two exceptions which are both (Mg^{2+}, Fe^{3+}) substituted are in the field of G s.d.

8.1.5. Basic alkali. (Table 8.1. Fig. 8.5).

The bulk of amphiboles from basic alkali host rocks, that is from basanites, trachyandesites, trachybasalts, camptonites, monchiquites, lugarites, essexites etc. form a discrete group of calcic amphiboles with Al^z in excess of 1.7 and high but variable Al^y (0.8 - 2.1). The majority of such amphiboles are kaersutites, the remainder also occur in the fields of Pa and Su s.d. Calcic amphiboles with lower Al^z which are from alkali gabbros 1643, 1644 (Onuki & Tiba 1964) and type shonkinites 1017, 1018 (Blyth & Lambert 1970) have either Tr of Ts as the dominant component of the basic atomic formula. Soda calcic amphiboles 1319, 1320 in R s.d. and 1321 in Ec s.d. are replicate analyses from an altered uncompahgrite (Larsen 1938, 1942). The alkali amphibole 2258 (Vlasov

et al. 1966) in Ec s.d. is from an urtite. Like the amphiboles from ultramafic - ultrabasic host rocks the basic atomic formulae are (Mg^{2+}, Fe^{3+}) and (Mg^{2+}, Al^{VI}) substituted.

8.1.6. Alkali. (Table 8.1. Fig 8.6).

Amphiboles from alkali igneous host rocks form two discrete groups, (i) those with Al^{Z} in excess of 1.6 including both calcic, and soda calcic amphiboles, and (ii) those with Al^{Z} less than 0.9 from the calcic, soda calcic and alkali amphiboles. Amphiboles from the former category are predominantly Pa s.d. with less common Su, Ts s. d. and kaersutites, and are typically (Fe^{2+}, Fe^{3+}) substituted.

Amphiboles from the low Al^{Z} category fall predominantly in the field of Ec s.d. and less commonly G, R,Tr and M s.d. The miyashiroite, 2241 (Volkov et al. 1962) has been discussed previously (Section 5.4.1). The three low Al^{Z} calcic amphiboles, 866 from a nepheline syenite (Heron 1924), 2356 from a druss in syenite (Zambonini 1905) and 2563 from a fenitised quartzite (Woolley et al. 1970) are all in Tr s.d. 592 from a syenite (Erdsmannsdorffer 1929) is the fourth Tr s.d. Basic atomic formulae of the low Al^{Z} category are variously (Mg^{2+}, Fe^{3+}), (Fe^{2+}, Fe^{3+}), (Mg^{2+}, Al^{VI}) and (Fe^{2+}, Al^{VI}) substituted.

8.2. Amphiboles from metamorphic host rocks.

The basic atomic formulae of amphiboles from metamorphic host rocks are both more numerous and more varied than those from igneous occurrences.

8.2.1. Calcareous metamorphic host rocks.

Inspection of Figs 7.1 - 7.28 and Table 8.1 suggests, as might be expected, that most amphiboles from calcareous metamorphic parageneses are calcic. For clarity the calcic amphiboles have been included on one figure. Inspection of Fig. 8.7 shows that calcic amphiboles from marbles and skarns form two groups, one near tremolite which is

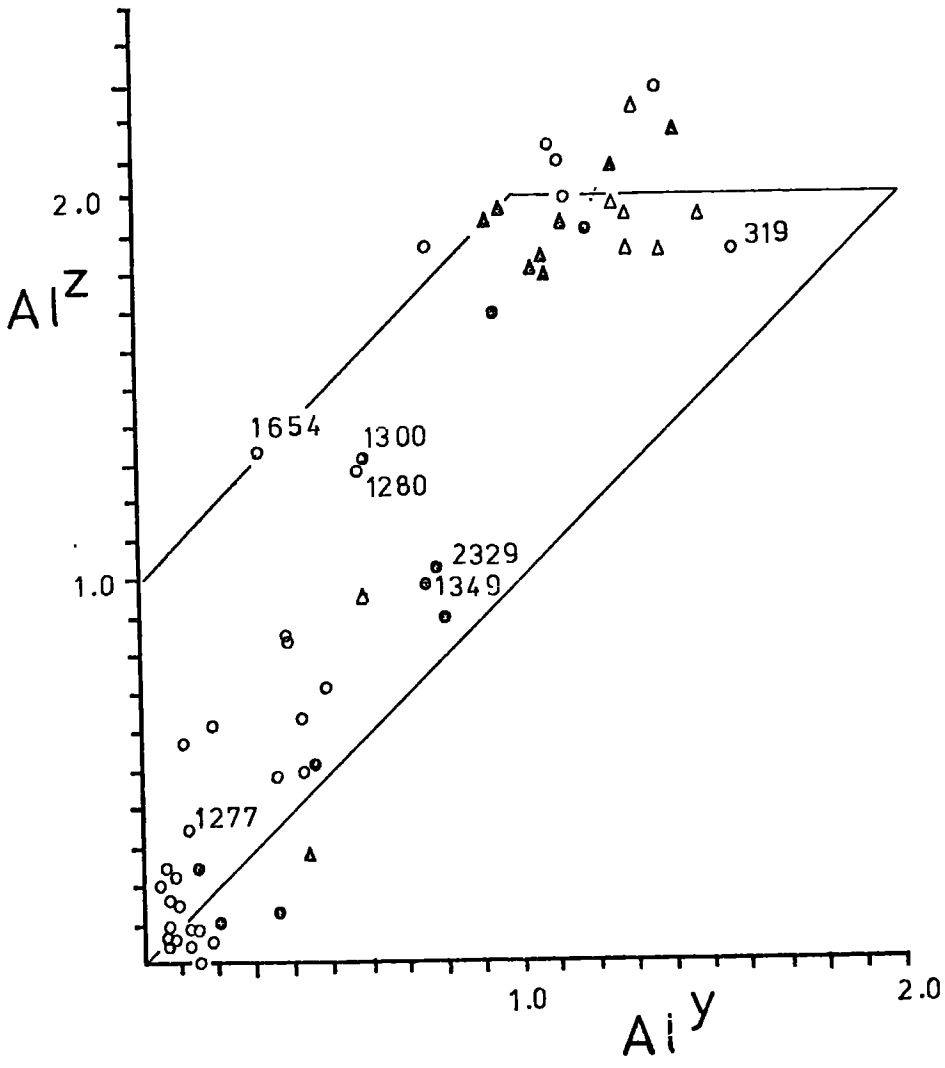


Fig. 8.7. Al^Z versus Al^Y in calcic amphiboles from metamorphosed calcareous host rocks. Symbols are the same as Figs. 8.1 - 8.6.

characteristically (Mg^{2+}, Al^{vi}) or (Mg^{2+}, Fe^{3+}) substituted and the second near pargasite which is more varied in Mg^{2+}-Fe^{2+} and Al^{vi}-Fe^{3+} substitution. Only seven calcic amphiboles, numbered on Fig. 8.7 do not plot either in Tr or Pa s.d. One of these, 319, (Buerger 1927) in Ts s.d. without K_2O or Na_2O must be considered inferior. The remaining six, 2329 (Winchell 1931), and its replicate analysis, 1349 (Leake 1962) from Eganville, 1280 (Kreutz 1908), 1300 (Laitikari 1920) from Pargas, 1654 (Palache 1935) from Sterling Hill, New Jersey, and 1277 (Kreutz 1908) from Russell, New York all in Ed s.d. appear to be satisfactory.

Not all the amphiboles from calcareous parageneses are calcic. Also included in Figs 7.1 - 7.28 are three soda calcic amphiboles from manganiferous skarns (1833, Rondolino 1936; 2810 Sundius 1946; 1213 Klein & Ito 1968) and three alkali amphiboles (1316, 1317, 1318 Larsen 1938) from carbonate bodies associated with alkali igneous rocks (Larsen 1938, 1942). The first three lie in the fields of Tr, R and G s.d. respectively and the latter three are all in Ec s.d. Drysdall & Newton (1960) have described an asbestiform amphibole associated with dolomite from Lusaka, Zambia, but both the analyses of the material, 482, 483, failed to give a balanced basic atomic formula. If amphiboles from calcite bearing hydrothermal veins are included there are a further three soda calcic amphiboles in Figs 7.1 - 7.28. These are 1311, 1313, (Larsen 1938), which were included in the ultramafic - ultrabasic category on Figs 7.1 - 7.28 and Table 8.1, 2832 (Larsen 1942) in R s.d. and 682 (Foshag 1936) with G as the dominant component.

8.2.2. Ferruginous metamorphic host rocks.

From Figs 7.1 - 7.28 it can be seen that amphiboles from ferruginous metamorphic parageneses plot in the FeMgMn, calcic or alkali amphiboles. FeMgMn amphiboles all have low Al^z (< 0.10) and display varying

degrees of Fe^{2+}, Mg^{2+} substitution. All are apparently monoclinic and therefore are cummingtonite - grunerites. The calcic amphiboles all plot in the field of Tr s.d. (Table 8.1) and with a single exception, 582 (Bonnischen 1969), have Mg^{2+} in excess of Fe^{2+}. This analysis also differs in having an Al^{z} of 0.77; all the other tremolites from ironstones have Al^{z} less than 0.30. The alkali amphiboles are (Fe^{2+}, Fe^{3+}) substituted and plot close to G. There is in addition a single (Mg^{2+}, Fe^{3+}) substituted soda calcic amphibole, 2562 (Klein 1966) in G s.d. This and 2661, also from an ironstone but which does not give a balanced basic atomic formula, have been discussed in Section 7.2.

Recently a considerable number of additional analyses lacking H_2O^+, F or Cl have been published (Mueller 1960; Krank 1961; Bonnischen 1969; Annersten & Ekström 1971). Examination of these analyses does not markedly affect the above statements except that the range of Al^{z} in the calcic amphiboles is increased to 1.21 by 581, (Bonnischen 1969).

8.2.3. Serpentinite metamorphic host rocks.

Very little can be said regarding amphiboles from serpentinites as there are only six included in Figs 7.1 - 7.28. Four of these are calcic with a wide range of Al^{z} (0.44 - 1.94) and Al^{y} (0.42 - 1.00) and plot in the fields of Tr, and Pa s.d. (Table 8.1). There is one soda calcic amphibole, 1341 (Laudermilk & Woodford 1930), which was originally considered to be orthorhombic but was later shown by Rabbit (1948) to be monoclinic. There is also a single FeMgMn amphibole which is apparently orthorhombic and plots close to Anth. As might be expected all are (Mg^{2+}, Al^{vi}) substituted.

In the data base as a whole there were only a further six analyses from serpentinites and these were either FeMgMn or calcic amphiboles.

8.2.4. Eclogites.

Inspection of Figs 7.1 - 7.28 and Table 8.1 shows that basic atomic formulae of amphiboles from eclogite host rocks while characteristically (Mg^{2+}, Al^{VI}) or (Mg^{2+},Fe^{3+}) substituted are varied in composition and include examples from the calcic, soda calcic and alkali amphiboles in the fields of Pa, Ts, Su, Tr, G s.d. and one kaersutite. The possible significance of this observed variation is discussed in Section 8.3.6.

8.2.5. Remaining metamorphic host rocks.

Included in this large category are those amphiboles from contact and regional metamorphic facies other than 'eclogite', calcareous, ferruginous or serpentinite host rocks.

As might be expected the basic atomic formulae of amphiboles from such diverse occurrences are highly varied and include examples from the calcic, soda calcic and alkali, FeMgMn and unnamed regions of amphibole compositional space and extended amphibole compositional space (Figs 7.1 - 7.28, Table 8.1). By far the largest proportion of these analyses are calcic with a pronounced maximum at Al^{Z} 1.6 (Figs 7.21 - 7.24, 7.29). These are subsiduary concentrations near G (Fig 7.1) and in the FeMgMn amphiboles (Figs 7.27, 7.28).

In terms of sensu dominante nomenclature amphiboles from such metamorphic host rocks are predominantly in the fields of Ts, Pa, and Tr s.d. with fewer analyses in G, Ed, Su, and M s.d. In contrast to the basic atomic formulae of amphiboles from igneous rocks there are a number of apparently reliable analyses in Ed s.d. but none with R or Ec as the dominant component, and no kaersutites.

The calcic, soda calcic and alkali amphiboles are characteristically (Mg^{2+}, Al^{VI}) or (Mg^{2+}, Fe^{3+}) substituted. This is partic-

ularly evident in the case of the low Al^{z} calcic amphiboles in the fields of Tr and Ed s.d. where Mg^{2+} excedes Fe^{2+} in almost every instance. However, ferrous substituted amphiboles are not entirely absent with (Fe^{2+}, Al^{vi}) and (Fe^{2+}, Fe^{3+}) substitution being found concentrated in the fields of Ts and Pa s.d. respectively. Lastly amphiboles in the FeMgMn and unnamed region of extended amphibole compositional space are similarly (Mg^{2+}, Al^{vi}) or (Mg^{2+}, Fe^{3+}) substituted.

8.3. Discussion of the observed relationships between amphibole composition and mode of occurrence.

From the preceding description of the distribution of basic atomic formulae illustrated in Figs 7.1 - 7.28 it is apparent that when considered together amphiboles from igneous and metamorphic host rocks are distinctive in a number of aspects. Thus for example, igneous amphiboles with edenite as the dominant component or plotting in the FeMgMn amphiboles are uncommon compared with amphiboles from metamorphic host rocks, while the reverse situation applies to R, Ec s.d. and kaersutite. After allowing for the fact that some of these features may be related to sampling bias in the illustrated analyses a number of tentative suggestions are made below which may explain these observed differences. Further an attempt is made to explain qualitatively the extent of variation exhibited by amphiboles within single amphibole host rock categories and between related categories.

8.3.1. FeMgMn amphiboles from igneous host rocks.

Perhaps the most striking difference between the observed distribution of amphiboles from igneous and metamorphic host rocks is the apparent scarcity of igneous FeMgMn amphiboles. Only three are illustrated in Figs 7.1- 7.28. Of these 2838 (Savolahti 1966) occurs as a late stage alteration product of orthopyroxene in a gabbro while

1014 (Bowen & Schairer 1935) which is from a fayalite bearing granite pegmatite may have formed by late stage reaction between quartz and fayalite (Ernst 1968). The third FeMgMn amphibole, 302 (Buckley & Wilkins 1971) occurred as phenocrysts in ryholite pumice breccia. In addition to these analyses cummingtonite has been recorded from basic igneous rocks where it is secondary after orthopyroxene and frequently associated with a calcic amphibole (Deer 1935; Nockolds 1941; Seitsaari 1952; Shido 1958). More recently the occurrence of phenocrysts of cummingtonite plus calcic amphibole in rhyolite and dacite lavas has been recognised (Kuno 1938; Klein 1968; Ewart et al. 1971, 1975).

Schurmann (1968) found that the upper thermal stability of amphibole in the join cummingtonite - grunerite at 1 kb ranged from 595° C to greater than 660° C. This relatively low upper stability may account in part for the apparent scarcity of primary igneous cummingtonite - grunerite. This is consistent with the observations of Ewart et al. (1975) who found that of the mafic phenocryst assemblages from the Taupo ryholites, those with cummingtonite had the lowest equilibration temperatures in the range 725 - 755° C at 1 - 3 kb. The presence of olivine plus quartz as the high temperature assemblage equivalent to grunerite (Schurmann 1968) is also consistent with the petrographic observation that grunerite from Rockport Mass. (Bowen & Schairer 1935) formed by reaction between olivine and quartz. It is suggested therefore that the relative scarcity of primary igneous cummingtonite - grunerites reflects the relatively low thermal stability of the series. A similar explanation may account for the apparent lack of primary gedrite (Hinrichsen 1968) but not anthophyllite (Greenwood 1963). Presumably in the case of anthophyllite, and for that matter cummingtonite and gedrite, factors such as host magma composition, P_{H2O} and the ease with which the mineral can be identified are important in explaining the apparent absence of such amphiboles

from igneous rocks.

8.3.2. Igneous amphiboles with edenite as the dominant component

With one exception there are no igneous amphiboles illustrated in Figs 7.1 - 7.28 near edenite or with Ed as the dominant component of the basic atomic formula (Table 8.1). While it is possible that this may be attributed to a bias in sampling it is worthy of note that Leake (1971) noted a similar feature in an independant collection of analyses. However, inspection of Table 8.1 shows that amphiboles with Ed as the dominant component are found in calcareous and general metamorphic parageneses but are also absent from eclogites. The stability field of edenite and ferro-edenite have not, as far as the author is aware, been determined, although edenite and ferro-edenite have been synthesised at 850° C, 2 kb and 600° C, 3 kb respectively (Colville et al. 1966). Leake (1971) considered that the absence of igneous amphiboles near edenite and ferro-edenite could be attributed to a rather low thermal stability of both phases. The evidence presented here of the almost complete lack of such compositions from igneous and eclogite parageneses is not inconsistent with such an interpretation.

8.3.3. Kaersutite.

Inspection of Table 8.1 shows that kaersutite is almost exclusively confined to igneous parageneses. The sole exception, 2305 (White et al. 1972) is from an 'eclogite' nodule associated with the nephelinite breccia, Kakanui, New Zealand. Taking the entire amphibole data file a further five kaersutites from 'eclogite' paragenese were located. Two of these were also from Kakanui, 1442, 1444 (Mason 1968a,b) and three were from Lherz in France, 1493 (Mottana Edgar 1969), 2399, 2400 (Conquere 1971) where they occur in dykes or layered differentiates in lherzolite. Only three other

amphiboles with Ti^{4+} in excess of 0.5 atoms in the amphibole data file were reported from metamorphic host rocks. Two of these, 1565, 1566 (Naidu 1954) were considered to be inferior analyses and did not comply with the definition of kaersutite, see Section 5.5.1. The third analysis, 650 (Fabries 1963) which is from an amphibolite, while complying with the definition of kaersutite is suspect in not achieving charge balance and has 0.48 atoms of Ca^{2+} in the A-site. Thus with the exception of those from 'eclogites' the remaining kaersutites in the amphibole data file for which paragenese are known are all from igneous rocks.

Of the igneous kaersutites, 850, 851 and 855 (Hermes 1970) which occurred in a two pyroxene gabbro and 2662 which crystallised from olivine tholeiite starting material (Holloway & Burnham 1972) are exceptional in being from tholeiitic rock types. All four are electron microprobe analyses with Ti^{4+} only marginaly in excess of 0.5 atoms and all iron reported as FeO which tends to exaggerate the numerical value for the cations including Ti^{4+} (see Chapter 3). Closer examination of the mode of occurrence of the remaining kaersutites allows three broad categories to be recognised.

(1) Alkali rich, silica undersaturated, often feldspathoidal plutonic igneous rocks including, teschenite (Aoki 1963), lugarite (Howie 1963), alkali gabbro (Frisch 1970; Valiquette & Archambault 1970; Borley et al. 1971; Ridley 1971), essexite (Adams 1903; Harrington 1903; Bancroft & Howard 1923) minverite (Kempe 1968), lherzite (Conquere 1971), camptonite, monchiquite (Kaiser; Campbell & Schenk 1950; Vincent 1953), syenite, pulaskite (Mauritz 1911; Wolff 1929; Streckeisen 1954; Bose 1963; Perchuk et al. 1967; Frisch 1970), monzonite, monzodiorite (Novotny 1949; Yagi 1953; Frisch 1970; Valiquette & Archambault 1970).

(2) Phenocrysts in alkali rich silica undersaturated extrusive rocks including, trachybasalt, trachyandesite (Harumoto 1933; Kawano 1934; Wilkinson 1961; Aoki 1963; Uchimuzu 1966), phonolite (Borley et al. 1971) and a number from unspecified basic rock types (Schneider 1891; Washington & Wright 1908; Tomita 1962; Borley et al. 1971).

(3) Xenocrysts and xenoliths in rocks of the former two categories, including xenocrysts (Aoki 1963; Wise 1966; Mason 1968a; Binns 1969; Aoki 1970; Best 1970), gabbroic (plagioclase bearing) xenoliths, (Aoki 1959; LeMaitre 1969; Aoki 1970; Best 1970), ultrabasic (combinations of the phases amphibole, clinopyroxene, olivine, spinel, rare orthopyroxene) xenoliths (Frisch & Schminke 1969; Aoki 1970; Best 1970; Prinz & Nehru 1970; Borley et al. 1971; Laughlin et al. 1971) and syenite xenoliths (Borley et al. 1971).

It is apparent therefore that kaersutite, including those from 'eclogites' are confined to, or associated with, silica undersaturated, often alkali rich and feldspathoidal plutonic or extrusive igneous parageneses. With the data available it has not been possible to define those criteria which determine the occurrence of kaersutite although it is evident from the observed occurrences that appropriate physical conditions are not attained during regional or contact metamorphism except in some eclogites themselves associated with igneous rocks. In this connection it is of interest to note that unpublished experimental work by Tuthill and Irving quoted in Kesson & Price (1972) suggested that kaersutite occurred both as a subsolidus phase and coexisted with melt in basic alkali compositions under hydrous conditions at 25 - 30 kb. Yagi et al. (1969) indicated that kaersutite was stable between 1 atm and 30 kb.

8.3.4. Metamorphic amphiboles with richterite and eckermannite as the dominant component.

Compared with amphiboles from igneous parageneses those from metamorphic parageneses show a smaller proportion of amphiboles with either R or Ec as the dominant component of the basic atomic formula. Of the metamorphic amphiboles included in Table 8.1, R and Ec s.d.

are confined to calcareous and serpentinite parageneses, although the serpentinite richterite (1341 Laudermilk & Woodford 1930) occurred in a hydrothermal vein. A search of the entire amphibole data file for R and Ec s.d. from other than calcareous metamorphic parageneses located only one further richterite (1193, Klein 1969) and two eckermannites (1180, Klein 1969; 2237 Palache 1894). The richterite has been discussed previously in Section 7.2.1. 1180 is an electron microprobe analysis. Recalculation of an optimum iron oxidation state moves the basic atomic formula into G s.d. for reduced iron ratios less than 0.8. The second eckermannite was re-analysed by Borg (1967b) as 209 and plots in G s.d. There would appear therefore to be no reliable analyses in the amphibole data file from a non-calcareous metamorphic paragenesis with Ec as the dominant component.

The reason for the scarcity or absence of amphiboles with R or Ec as the dominant component from these non-calcareous parageneses is normally attributed to the unusual chemical requirements of these amphiboles (Phillips & Rowbotham 1968). This is emphasised by the high thermal stability of richterite, ferro-richterite (Charles 1972) and eckmermannite (Phillips & Rowbotham 1968).

8.3.5. Variation in composition of igneous amphiboles with mode of occurrence.

While the range of Al^z in the calcic amphiboles in each of the six igneous host rock categories is large the lower limit decreases steadily in passing from ultramafic - ultrabasic through basic and

intermediate to acid igneous rocks. This is also apparent in the increasing number of analyses in Tr s.d. (Table 8.1). Leake (1971), following Harry (1950) interpretated the variation in Al^z (Al^{iv}) of amphiboles from igneous rocks as reflecting their temperature of crystallisation. However, the high Al^{iv} in amphiboles from basic alkali and alkali parageneses suggests that the variation is also related to the availability of silica in the magma. This does not imply that Al^{iv} is independant of temperature but rather that variation due to temperature is likely to be most important in amphiboles crystallised from similar bulk compositions over a range of physical conditions as in the case of metamorphic rocks.

Experimental phase equilibria studies of pargasite (Boyd 1959; Holloway 1973), ferro-pargasite (Gilbert 1966) and ferri-pargasite (Semet 1973) showed that under appropriate chemical and fO_2 conditions all three amphiboles were stable at magmatic temperatures. In the presence of excess SiO_2 the stability of pargasite and ferro-pargasite were found to be markedly reduced and because of the presence of olivine and nepheline, both undersaturated with respect to silica, in the high temperature assemblage of ferri-pargasite the addition of SiO_2 should lower the thermal stability of this amphibole also. It is of interest to note therefore that (Mg^{2+}, Al^{vi}), (Mg^{2+}, Fe^{3+}) and (Fe^{2+}, Al^{vi}) substituted amphiboles with Pa as the dominant component occur most abundantly in ultramafic - ultrabasic, basic, intermediate and basic alkali host rocks and only relatively infrequently in acid and alkali igneous host rocks where amphiboles with Pa as the dominant component are typically (Fe^{2+}, Fe^{3+}) substituted (Table 8.1). It is suggested therefore that ferri-ferro-pargasite (hastingsite) may be stable in the presence of excess SiO_2.

Factors other than the availibility of silica must be invoked

to explain the low and high Al^{z} amphiboles from acid and alkali igneous host rocks. The ratio of aluminium to alkalis is probably important. Thus if titanium is absent all amphiboles plotting on the high Na^{X} side of a plane through Tr, Ed, M, G in amphibole compositional space are peralkaline irrespective of ferric-iron substitution for Al^{vi} and those on the high Na^{X} side of the plane through Tr, Ed, Su, Ts_{50} G_{50} can be peralkaline if Al^{vi} is replaced by Fe^{3+}. All the low Al^{z} soda calcic and alkali amphiboles from acid and alkali parageneses as well as the calcic amphiboles 868, 2563 fall in these regions of amphibole compositional space.

As in the other mafic silicates the amphiboles show the replacement of Mg^{2+} by Fe^{2+} in passing from ultramafic - ultrabasic to acid and basic alkali to alkali rock types. At the same time Al^{3+} is reduced and Al^{vi} is progressively replaced by Fe^{3+} probably in response to decreasing Al^{3+} content and increasing water and hence iron oxidation state in the magma.

8.3.6. Variation in composition of metamorphic amphiboles with mode of occurrence.

Without a knowledge of host rock composition and metamorphic facies very little can be inferred regarding the relationship between amphibole composition and mode of occurrence.

The bimodal distribution of calcic amphiboles from calcareous host rocks is similar to those recognised by Hallimond (1943) and Leake (1968, 1971). Hallimond considered that amphiboles near tremolite formed by isochemical metamorphism of impure limestones while the formation of those near pargasite involved the introduction of alkalies.

In Section 8.2.4, amphiboles from eclogites were found to be highly variable in composition. This is perhaps surprising from a

rock type which has been given metamorphic facies status (Turner 1968), although the commonly observed retrogression of eclogites may be important in this respect. Because of this observed variation and the relatively small number of analyses involved a more detailed study of eclogite amphiboles was undertaken. The status of the names barroisite and carpinthine used frequently for amphiboles from eclogites is also discussed.

Eclogites may be defined, in a non-genetic way, as rocks of basaltic composition, consisting of essential Mg^{2+}-Fe^{2+} garnet plus clinopyroxene (Lovering & White 1969). Other primary phases which can occur include amphibole, epidote, kyanite, quartz, orthopyroxene and rutile. Primary plagioclase is normally excluded (Green & Ringwood 1967; Winkler 1967 but cf Coleman et al. 1965). Eclogites tend to occur in small bodies associated with, and often tectonically emplaced within, metamorphic rocks of diverse character. Coleman et al. (1965) subdivided eclogite occurrences into three categories (i) as inclusions in kimberlites, basalts or layers in ultramafic rocks - Type A, (ii) as bands of lenses in migmatite gneiss terrains - Type B and (iii) bands or lenses associated with glaucophane bearing schists - Type C. They found that the pyrope content of garnet and to a lesser extent the jadeite content of pyroxene varied systematically between eclogites of types A through B to C. Coleman et al. attributed this variation in phase chemistry to differing physical conditions during eclogite formation rather than to variation in rock bulk chemistry and suggested that eclogites could form over a wide range of pressure and temperature conditions. Extrapolation of experimental evidence of Green & Ringwood (1967) suggested that under anhydrous conditions the basalt - eclogite transformation can occur under conditions of the glaucophane lawsonite schist, albite epidote amphibolite and amphibolite facies. Field evidence of

interlayered eclogite and high temperature blueschists (Coleman et al. 1965) and eclogite and albite epidote amphibolite facies rocks (Morgan 1970) lends support to the theory of multiple origin of eclogites.

Mottana & Edgar (1969) showed that the Al^{vi} and Al^{iv} contents of amphiboles from eclogites were variable and this they suggested reflected variation of pressure and temperature of crystallisation respectively. However, there are a number of disquieting features of the data used by Mottana and Edgar. For example they included analyses which the original author explicitly stated were secondary (Sahlstein 1935; Alderman 1936; Bearth 1959; Borg 1967b), an analysis which occurred as a xenocryst and not in an eclogite (Dickey 1968), and analyses from plagioclase bearing assemblages (Knorring & Kennedy 1958; Livingstone 1967).

Because of the variation in basic atomic formulae of amphiboles from eclogites observed in Figs 7.1 - 7.28 and the significance of variations in compositions of primary minerals in eclogites with respect to mode of occurrence, a search of the complete amphibole data file for analyses from 'eclogites', 'amphibolitic eclogites', and other garnet pyroxene assemblages such as 'garnet pyroxenites', 'garnet ariegites', 'garnet websterites' was undertaken. As far as possible, analyses located in this way were subdivided into four categories.

(1) Inclusions in kimberlite, basic alkali lavas or tuffs, and lenses in ultramafic - ultrabasic intrusions.

(2) Associated with metamorphic rocks belonging to the amphibolite and granulite facies.

(3) Associated with metamorphic rocks belonging to the albite epidote amphibolite facies.

(4) Associated with glaucophane bearing schists.

Groups 1, (2 and 3) and 4 correspond respectively to type A, B and C eclogites of Coleman et al. (1965). Amphiboles from each group were further subdivided into those which apparently coexisted with garnet and clinpyroxene and were primary and those which were secondary. In addition assemblages with interstitial plagioclase have been separated. Lastly, amphiboles where there was insufficient information in the original reference to allocate to one of the above groups or to determine whether primary or not have been included in a fifth group.

Basic atomic formula Al^{z} verus Na^{x} for calcic, soda calcic and alkali and Al^{z} versus Al^{y} for calcic amphiboles from eclogites are illustrated in Fig 8.8, where the source of the data is also given. Where appropriate optimum iron oxidation states have been calculated and these are shown as bars linking appropriate symbols.

It is apparent from Fig 8.8 that the variation in composition of amphiboles from eclogites can not wholly be attributed to retrogression. Apparently primary amphiboles include examples from the calcic, soda calcic and alkali amphibole groups and show a strong relation to the mode of occurrence of the eclogite. Secondary amphiboles show a less well categorised distribution.

Primary amphiboles typical of group 1 occurrences are calcic with $Al^{z} > 1.8$ (except for 2800 (Shido 1959), 2813 (Ernst et al. 1970) both from the Higashi-akaishi-yama peridotite, Shikoku) and have either Pa or Su as the dominant component. The titanium content is variable. Three, 561 (Bloxam & Allen 1960), 2800, 2813 (Ernst et al. 1970) have $Ti^{4+} < 0.1$ atoms while the remainder all have $Ti^{4+} > 0.35$ atoms and include six kaersutites, three from Kakanui (1442, 1444 Mason (1968a,b), 2305 White et al. 1972)) and three from Lherz (1493 Mottona & Edgar 1969), 2399, 2400 (Conquere 1971)).

Fig. 8.8. Al^Z versus Na^X for calcic, soda calcic and alkali amphiboles(a) and Al^Z versus Al^Y for calcic amphiboles (b) from eclogites.

Group (1)

Primary ▼ 2800, Shido (1959); 561, Bloxam & Allen (1960); 1442, 1444, Mason (1968a,b); 1390, 1391 Lovering & White (1969); 1494, Mottana & Edgar (1969); 2813, Ernst et al.(1970); 2395, Meyer & Brookins (1971); 2305, White et al.(1972).

Plagioclase bearing ⓥ 1493, Mottana & Edgar (1969); 2399, 2400, Conquere (1971).

Group (2)

Primary ● 191, Koritnig (1940); 1611, O'Hara (1960); 2421, O'Hara & Mercy (1963); 2397, Mottana, Church & Edgar (1968);1495, 1496, Mottana & Edgar (1969); 2228, Velde et al.(1970); 299, Bryhini & Griffin (1971).

Secondary ○ 1972, Sahlstein (1935); 2, Alderman (1936); 843, Heritsch & Kahler (1960); 2307, 2309, 2310, 2312, 2314, Wiikström (1970).

Plagioclase bearing ◎ 1382, Livingstone (1967); 1491, 1497, Mottana & Edgar (1969).

Group (3)

Primary ■ 107 Banno (1964); 190 Binns (1967); 2812, 2814, 2815, Ernst et al.(1970); 1470 - 1473, Morgan (1970).

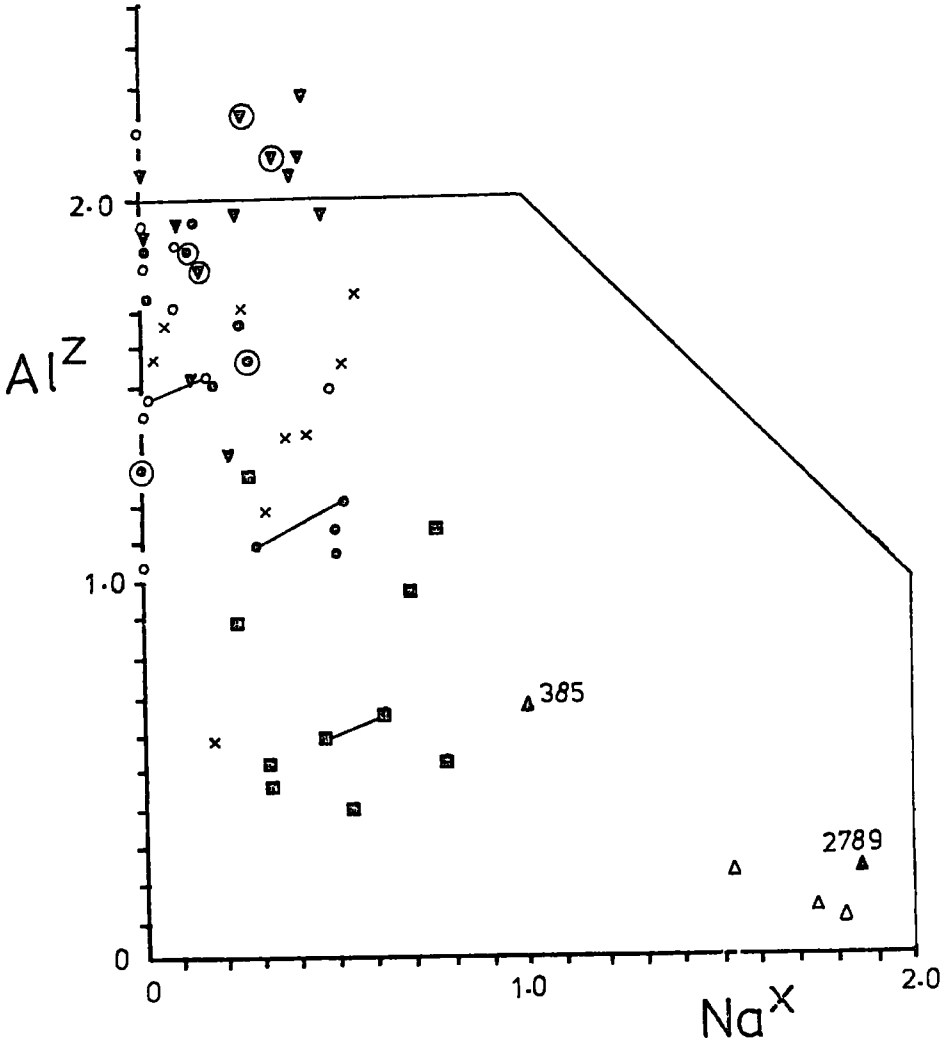
Group (4)

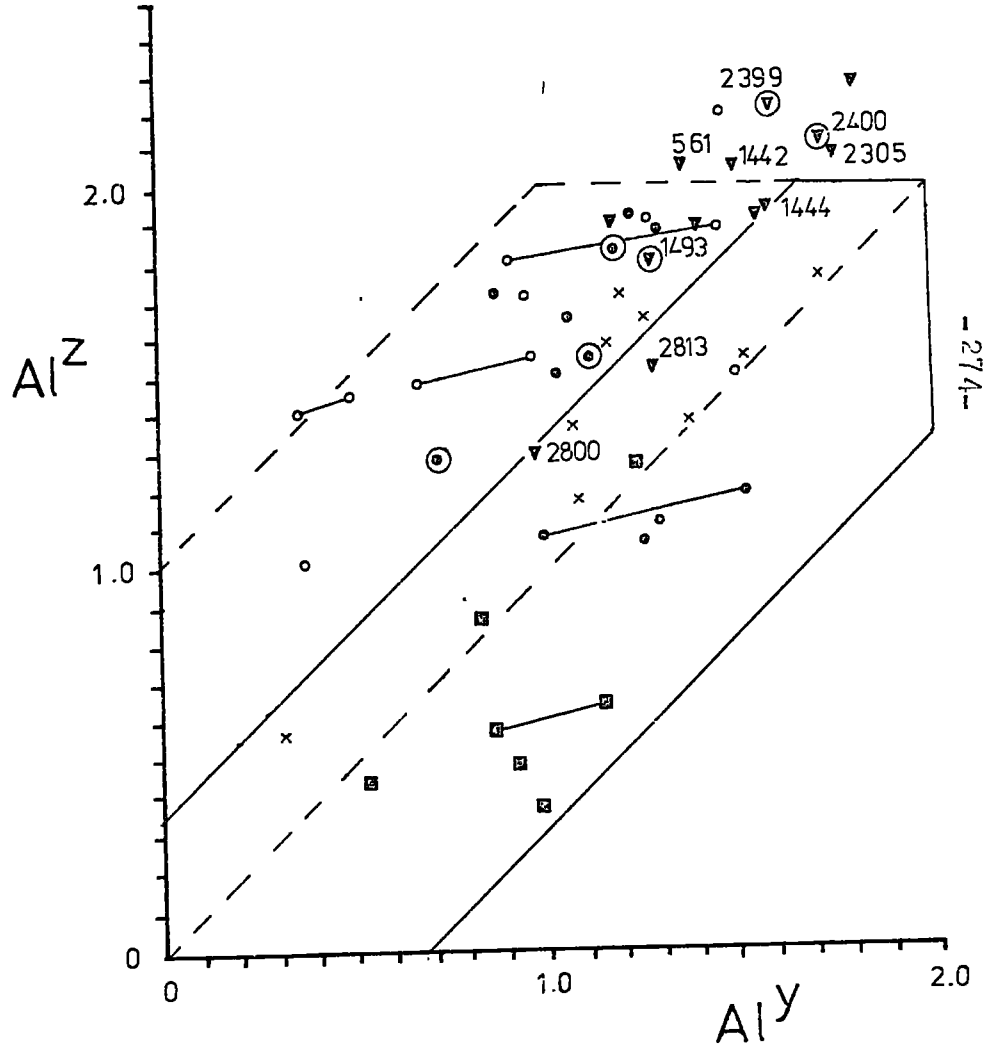
Primary ▲ 2789, Chesnokov (1960); 385, Coleman et al.(1965)

Secondary △ 142, Bearth (1959); 206, 207, Borg (1967b).

Group (5) ×

832, Hezner (1903); 1279, Kreutz (1908); 3, Eskola (1921); 2345, Wolff (1942); 548, Daniels (1956); 845, 846, Heritsch, Paulitsch Walitzi (1957); 844, Heritsch & Kahler (1960); 1414, Machatchski & Walitzi (1963).


2·0
1·0
0
0
1.0
2.0
Al^Z
Na^X
385
2789


2.0
1.0
0
0
1.0
2.0
Al^Z
Al^Y
2399
2400
561
1442
2305
1444
1493
2813
2800

Amphiboles from group 2 occurrences are calcic with Al^z 1.0 - 1.9 and have either Pa and less commonly Ts as the dominant component. The group 3 amphiboles are calcic and soda calcic with $Al^z < 1.3$ and with either Tr of Ts as the dominant component. Titanium in both these groups is less than 0.25 atoms.

Lastly, there are only two apparently primary amphiboles from group 4 occurrences. These are 385 (Coleman et al.1965) a soda calcic amphibole with Ts as the dominant component and 2789 (Chesnokov 1960) an alkali amphibole close to G. The latter comes from a garnet, emphacite, amphibole, epidote, quartz, muscovite, rutile assemblage which with other 'eclogite' assemblages of garnet, amphibole, omphacite, glaucophane, actinolite, and rutile reported by Chesnokov (1960) from the same region closely resemble the high-temperature blueschists of Taylor & Coleman (1969) some of which, for example, 2830 - 2831, 1171 - 1172 contained calcic and alkali amphibole pairs, see Section 7.2.2.

A plot of Al^{iv} verus Al^{vi} is given in Fig. 8.9 from which it can be seen that the differences between the primary amphiboles from differing modes of occurrence is maintained. It is tempting to correlate the variation of Al^{iv} and Al^{vi} with the temperature and pressure of crystallisation and to interpret the variation of Al^{iv} and to a lesser extent Al^{vi} in primary amphiboles as evidence of a range of temperatures and less obviously pressure during eclogite formation. Such an interpretation is supported by the decrease in Al^{iv} from Type 1 through 2 to 3 and 4 occurrences.

In detail it is difficult to defend the use of Al^{iv} and Al^{vi} as indicators of temperature and pressure since their values depend both on the total Al_2O_3 and SiO_2 in the mineral analysis and indirectly the composition of the host rock. The presence of a solvus between the calcic and alkali amphiboles would, if present, also complicate

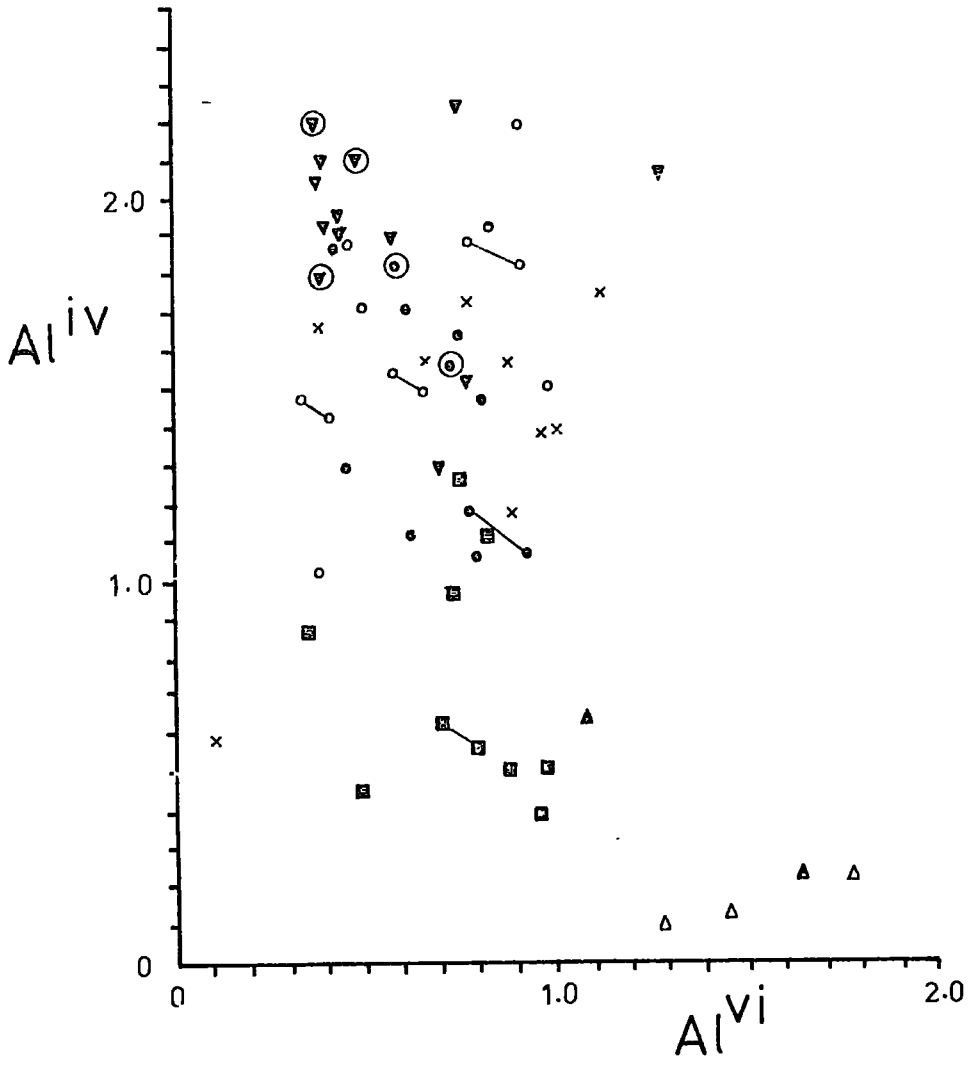


Fig. 8.9. Al^{iv} versus Al^{vi} in amphiboles from eclogites. Symbols and source of the data is the same as Fig. 8.8.

the interpretation. However, the large and systematic variation of basic atomic formulae of primary amphiboles from eclogites in terms of the mode of occurrence of the eclogites themselves, coupled with similar relationships reported for the garnets and clinopyroxenes, is consistent with eclogites having formed over a range of temperatures and pressures.

The present study does not answer the question of whether eclogites and amphibole bearing eclogites associated with rocks of various metamorphic facies, formed under the same pressure and temperature conditions as the rocks they are included in, but possibly with less water available (Taylor & Coleman 1969), or whether they represent different temperature and pressure conditions (Turner 1968).

The varietal names carinthine and barroisite have been used for amphiboles from eclogites, in particular those from type 2 and 3 occurrences. Koritnig (1940) and Binns (1967) suggested that both terms should be restricted to amphiboles from eclogites. To the present writer there is no reason for using these names since it seems unjustified to restrict a name to amphiboles from a single paragenesis, especially as the amphiboles from that paragenesis are remarkably varied.

9. SUMMARY AND CONCLUSIONS.

The variable composition and the occurrence of amphiboles in rocks belonging to a wide range of igneous and metamorphic parageneses makes the group potentially very valuable in interpreting the conditions under which their host rocks formed. Despite the large number of chemical analyses available for the amphiboles no such understanding has as yet emerged (Chapter 1). Three major factors have contributed to this situation. Firstly, the difficulty in deriving accurate atomic formulae from chemical analyses which stems from (i) the often incomplete nature of analyses, (ii) the presence of essential OH^-, F^- or Cl^- in the structure, (iii) the large number of alternative crystallographic sites or groups of sites, and (iv) the possibility of order - disorder with temperature of crystallisation. Secondly, the chemical complexity of the amphibole group which is reflected in the profusion of named amphibole varieties. Lastly, there is a lack of knowledge concerning the overall chemical variation exhibited by the group.

The aim of the present work has been to resolve these outstanding problems of amphibole mineralogy in order to relate, albeit in a very general way, amphibole composition and mode of occurrence. In order to achieve this a computer program to calculate atomic formulae and basic atomic formulae was written (Chapter 2) and a method devised to estimate the iron oxidation state in an analysis where this is unknown (Chapter 3). A simple graphical representation and rational nomenclature was devised for the amphiboles (Chapter 5) and used with a large computer data file of analyses (Chapter 4) to demonstrate the overall chemistry of the group (Chapter 7) and the relationship between amphibole composition and mode of occurrence (Chapter 8). The results drawn from this study and the conclusions

drawn from them are summarised briefly in the present Chapter.

9.1. Calculation of atomic formulae, basic atomic formulae and comparison of the 23(O) and 24(O) recalculation bases.

9.1.1. Allocation scheme.

An available computer program MINDATA3, written by R. Phillips, was evaluated by comparing the distribution of cations between groups of sites calculated from a chemical analysis alone with published experimentally determined cation distributions for the same analyses. The existing allocation scheme was found not to be entirely satisfactory (Section 2.1). Starting from published experimentally determined site populations (Appendix 3) and assuming that the observed ordering of cations between groups of sites reflected the preference of cations for groups of sites an amended allocation scheme was devised (Section 2.2). This was extended (Section 2.3) to include additional ionic species by further assuming that cations of similar ionic radius and charge would, if present, occupy similar co-ordination polyhedra. The derived allocation scheme (Section 2.4) was incorporated into a computer program entitled MINDATA5 (Appendix 4) To evaluate the allocation scheme calculated group populations were again compared with published experimentally determined cation distributions. Evidence presented in Section 2.5 of values near zero for the statistics $\bar{x}$, σ and $|\bar{x}|$ for Sa, Sb, Sc, and Sd which measured the difference between the calculated and experimentally determined group populations, plus evidence that with only seven exceptions values for Sb, Sd were consistently lower than those calculated using MINDATA3 was taken as indicating the superiority of the allocation scheme in MINDATA5 over that of MINDATA3.

For most purposes an atomic formula at group level is satisfactory. This greatly simplifies the calculation of the atomic

formulae since it is becoming increasingly apparent (Section 2.5) that variation of ordering of cations between the sites forming a group may in part be attributed to variation in physical conditions during crystallisation. In addition, Ghose & Weidner (1972) and Seifert & Virgo (1974) have reported experimental thermally induced variation in Mg^{2+}, Fe^{2+} ordering between the X and Y groups of cummingtonite and anthophyllite respectively. The additional variation in terms of Sb and Sd introduced by heating and subsequent quenching was found (Section 2.5) to be of similar magnitude to the discrepencies between the experimentally determined and calculated group populations noted above. However, it was considered unlikely that such large variations in ordering would be retained in more slowly cooled natural amphiboles and it was suggested that thermally induced variation of ordering between groups was small compared with the remaining discrepencies between experimentally determined and calculated site populations and could be neglected therefore.

In the light of future X-ray, Mössbauer and infrared site population determinations it may be possible to refine further the allocation scheme incorporated in MINDATA5. It may be possible to devise an allocation scheme for distributing cations between individual sites if a clearer understanding of the factors governing the distribution of cations between non-equivalent sites in a silicate lattice is forthcoming. In this connection lattice energy calculations assuming various electrostatic models have met with some success in predicting Fe^{2+}, Mg^{2+} distributions between non-equivalent sites in a number of ferromagnesian silicates (Burns 1970; Ohashi & Burnham 1972; Wood & Strens 1969).

9.1.2. Basic atomic formulae.

Atomic formulae to 23(O) and where appropriate 24(O) were

calculated for 2650 analyses contained in the amphibole data file (see Chapter 4). Simplified, or basic atomic formulae, were derived from the atomic formulae of these analyses using the method of Phillips & Layton (1964) incorporated into MINDATA5. Provided the analysis is accurate and the methods used in deriving the atomic and basic atomic formulae are correct the basic atomic charge balance equality $(Na^A + Al^Y) = (Na^X + Al^Z)$ should apply. In Chapter 6 it was demonstrated for the first time that approximate charge balance is achieved in the majority of analyses. Following Phillips' (1963) suggestion that in an accurate analysis the calculated group occupancies should be within 1 per cent of the number of lattice positions in the structural formula, $(Na^A + Al^Y) - (Na^X + Al^Z)$ should be less than $\pm$ 0.07. Some 60 - 67 per cent of analyses, calculated to 23(O), fall within these limits and this rises to 75 - 77 per cent if a wider range of $\pm$ 0.15 corresponding to an error of approximately 2 per cent is allowed. This latter value was taken as defining a balanced basic atomic formula. The achievement of charge balance in a large proportion of analyses does not prove the general applicability of the allocation scheme, nor the method used in deriving the basic atomic formula, but it is not inconsistent with such an interpretation.

It might be expected that in any large collection of analyses basic atomic formulae failing to achieve charge balance should be evenly distributed with respect to overall chemistry. However, the distribution of basic atomic formulae calculated to 23(O) over amphibole and extended amphibole compositional space illustrated in Figs 7.1 - 7.28 showed that analyses with $(Na^A + Al^Y) - (Na^X + Al^Z)$ in excess of $\pm$ 0.15 were concentrated into the low Al^Z portion of both spaces. A careful check was made of the transcription of these analyses and of the atomic formulae in order to try and find any

common features which may explain the discrepencies. However none were found. An error in the allocation scheme affecting oxyamphiboles (calculated to 24(O)) was found in Chapter 5. This is discussed below. Section 9.1.3.

9.1.3. Comparison of the 23(O) and 24(O) recalculation bases.

Taking only those analyses with either H_2O+, F or Cl determined the extent of charge balance in basic atomic formulae calculated to 23(O) and 24(O) were compared in Chapter 6. When calculated to 24(O) between 38 - 46 and 45 - 56 per cent had $(Na^A + Al^Y) - (Na^X + Al^Z)$ less than $\pm$ 0.07 and $\pm$ 0.15 respectively compared with values of 60 - 63 and 74 - 75 per cent of the same analyses to 23(O). Inspection of the more highly unbalanced basic atomic formulae revealed that many had $OH^- + F^- + Cl^-$ less than 2.0 and suggested that either the method used in MINDATA5 for balancing O^{2-} in oxyamphiboles was incorrect or alternatively that water and fluorine determinations in a considerable number of analyses were suspect.

Phillips (1963) suggested that O^{2-} in the hydroxyl group was balanced solely by Fe^{3+} according to the substitution $Fe^{3+} + O^{2-} = Fe^{2+} + OH^-$. This Phillips incorporated into MINDATA3, reducing Fe^{3+} by an amount equal to the O^{2-} substitution, but only when Fe^{3+} equalled or exceeded O^{2-}. For want of any evidence to the contrary this logic was also incorporated into MINDATA5 (Chapter 2).

Examination of the titaniferous amphiboles (Section 5.5.1) showed a negative linear relationship between iron oxidation state and $OH^- + F^- + Cl^-$ content consistent with the experimentally observed oxidation reaction $Fe^{3+} + O^{2+} = Fe^{2+} + OH^-$ (Yagi et al. 1969). Interestingly, in only three of the kaersutites was sufficient ferric iron available to balance the O^{2-} present. This was not because there was insufficient iron available, nor did it seem likely to be due to

undetermined F or Cl, or indicate alternative charge balancing substitutions of the type $Ti^{4+} + O^{2-} = Ti^{2+} + OH^{-}$. This feature could however be attributed to inaccurate, i.e. low, water determination (cf Leake 1965a).

In any case it was apparent that the charge balancing substitution should be made even when Fe^{3+} is less than O^{2-} and so in Chapter 6 the amount of ferric iron involved in such analyses was deducted from the value for Al^{Z} and new distributions of $(Na^{A} + Al^{Y}) - (Na^{A} + Al^{Z})$ calculated. There was only a marginal improvement of 2 and 4 per cent within $\pm$ 0.07 and $\pm$ 0.15 respectively. It would appear therefore that when considering large numbers of amphiboles of mixed analytical quality that a recalculation base to 23(O) is more likely to yield balanced basic atomic formulae than a 24(O) recalculation base.

9.2. Estimation of the iron oxidation state in electron microprobe analyses of amphiboles.

In order to estimate the iron oxidation state in electron microprobe analyses a method was devised in Chapter 3 which involved varying the Fe_2O_3 and FeO content of an analysis (total iron constant) until the basic atomic formula equality is achieved.

9.2.1. Theoretical atomic formulae with known oxidation states.

Starting from a number of Li^{+} and Ti^{4+} free atomic formulae with known oxidation states it was shown (Section 3.1), after first converting all iron to equivalent FeO and neglecting water, that the iron oxidation state (or reduced iron ratio) consistent with $(Na^{A} + Al^{Y}) = (Na^{X} + Al^{Z})$ can be either unique, or alternatively show a limited or complete range of values (Fig. 3.1). In each instance the estimated reduced iron ratio equalled or included the original 'correct' ratio. In order to explain these differences the derivation

of basic atomic formulae was considered in greater detail (Section 3.1.1) and a notation developed (Section 3.1.2) to describe the variation in the components of basic atomic formulae with varying reduced iron ratio. Using the notation it was shown (Section 3.1.3) that the range of reduced iron ratios for which ($Na^{A} + Al^{Y}$) equals ($Na^{X} + Al^{Z}$) varied systematically with the location of atomic formulae in amphibole compositional space. It was found that for most basic atomic formulae, ($Na^{A} + Al^{Y}$) equals ($Na^{X} + Al^{Z}$) for all reduced iron ratios. It was apparent therefore that the method in its simplest form would be unsuitable for estimating the iron oxidation state in all but a few special instances. By assuming that the substitution $2Fe^{3+} + \square = 3Fe^{2+}$ was inappropriate it was found that Li^{+}, Ti^{4+} free (Section 3.1.3) and Li^{+}, Ti^{4+} bearing (Section 3.1.4) theoretical atomic formulae yielded either unique or limited ranges of reduced iron ratios in each instance equal to or including the original ratio (Fig 3.1, 3.3). Further this applied to all portions of amphibole compositional space. The sole exception was analysis 20 (Fig 3.3) in which the substitution actually was present (Table 3.2). The range of reduced iron ratios could be limited further in some instances by applying a number of crystal chemical constraints (Fig 3.1, 3.3).

It is apparent therefore that using the equality of the basic atomic formula and where appropriate assuming the substitution $2Fe^{3+} + \square = 3Fe^{2+}$ is not applicable and applying crystal chemical constraints an accurate although frequently non-unique estimate of the iron oxidation state can be made. When compared with alternative stoichiometric estimates (Section 3.1.5) only the cation base Y + Z = 13 ($\sum FM = 13$, Stout 1972) was at all satisfactory, but this unlike the basic atomic formula method is limited to amphiboles with full Y group occupancy. Both methods are restricted to amphiboles within amphibole compositional space viz. $Na^{+} + Ca^{2+}$ in ≥ 1.95 atoms (see Chapter 5).

9.2.2. Actual analyses with known oxidation states.

A number of hydroxy amphiboles with known oxidation states and with basic atomic formula $(Na^A + Al^Y) - (Na^X + Al^Z)$ less than $\pm$ 0.01 were taken at random from the amphibole data file. Estimates of the iron oxidation state (in terms of reduced iron ratio) were made for these analyses using both the basic atomic formulae and stoichiometric methods and compared with the actual value (Section 3.2). While the resulting range of reduced iron ratios did not in general coincide uniquely with the original value they were consistent with it, (Fig 3.6). In contrast none of the stoichiometric bases yielded accurate or consistent results (Fig 3.7): the $\sum FM=13$ base giving oxidation states which were too low (more ferrous rich) than the actual value.

It may be argued that by choosing analyses with basic $(Na^A + Al^Y) - (Na^X + Al^Z)$ less than $\pm$ 0.01 an unrepresentative sample was taken, cf Chapter 6. However, inspection of Figs 3.1, 3.3, shows that taking the value of $\pm$ 0.15 as indicating charge balance does not markedly affect the resultant range of reduced iron ratios because of the generally steep negative slope in $(Na^A + Al^Y) - (Na^X + Al^Z)$ when the substitution $2R^{3+} + \square = 3R^{2+}$ is neglected. It would appear that the basic atomic formula method, while not yielding unique results is as good as, and probably superior, to alternative stoichiometric estimates of the iron oxidation state. The method was applied successfully to a number of apparently coexisting amphibole pairs in Chapter 7, and in Chapter 8. One interesting corallary of the range of reduced iron ratios over which $(Na^A + Al^Y)$ equals $(Na^X + Al^Z)$ is that the existence of a balanced basic atomic formula in an electron microprobe analysis with all iron reported as FeO (reduced iron ratio = 1.0) does not necessarily mean that there is trivial Fe_2O_3 present.

9.3. The amphibole data file.

Bearing in mind the large and rapidly expanding volumes of data relevant to the amphiboles (Fig 1.2) the need for a versatile computer data base capable of storing a comprehensive range of information in a form as close to the original as possible was envisaged (Chapter 4). To this end various data base strategies were considered. Available vector (FORTRAN and PL/1) and tree (PL/1) data base strategies were found to suffer from the disadvantages of data dependance and large scale data redundancy (Section 4.1). In order to reduce, although not eliminate, these drawbacks a data base was devised in which storage space was not allocated unless a response was actually present and any tree organisation could be used without altering the loading program (LOAD: Appendix 5) or the query program (QUERY: Appendix 5). The main disadvantages of the data base were that it was not particularly efficient in time and the method of adding data to LOAD was somewhat tedious. Both features could have been improved but a working prototype data base (Notley 1972) involving a relational model of data (Codd 1970; 1971) was kindly made available for the use by the writer in 1972.

The relational model of data which involved storing data in the form of relations (data tables with unique rows in which row ordering is immaterial) was found to be admirably suited for storing the contents of the amphibole data file. As far as the author is aware this is the first use of the relational model in the geological sciences although from the examples given in section 4.13 it is apparent that the model has great potential in coping with the often complex spatial and temporal inter-relationships present in many aspects of geological information (cf Dixon 1970).

Queries of the data base involve simple set operations (Appendix 6) and complete data independence is achieved (Roper, Osman &

Knight 1973). By a judicious choice of relations data redundancy can be reduced and if necessary a limited degree of hierarchical structuring can be maintained (Section 4.3). The amphibole data file implemented using the relational model of data was used extensively in assessing amphibole classification (Chapter 5), characteristics of basic atomic formulae (Chapter 6), the distribution of basic atomic formulae (Chapter 7) and the relation between host rock and amphibole composition (Chapter 8). The efficiency of the particular implementation of the relational model used here has been the subject of a study by Osmann (1974). The amphibole data file, in the form of punched cards grouped by relations and organised as described in Appendix 7 is lodged with Mr. R. Phillips, Dept. Geological Sciences, Univ. of Durham.

During data validification it was noted that published analytical and in particular optical data concerning amphiboles were frequently internally inconsistent.

9.4. Classification and nomenclature of the amphiboles.

In Chapter 1 Phillips' (1966) derivation of amphibole compositional space as a graphical representation and means of classifying the calcium and sodium rich amphiboles was described. Compared with alternative three dimensional representations proposed by Fabries (1966) and Leake (1968) amphibole compositional space was found to be superior in a number of aspects while the two dimensional representations of Hallimond (1943), Winchell (1945), Miyashiro (1957), Boyd (1959) and Leake (1968) can be considered as views of limited portions of the space (Section 5.1).

Phillips subdivision of amphibole compositional space into nine *sensu extensu* regions, each named after an apex or 'end member'

and each corresponding to regions in which greater than 50 per cent of an 'end member' component was present was found to be unsatisfactory. The regions did not in every instance correspond to greater than 50 per cent of an 'end member' component or to regions in which an 'end member' was dominant. An alternative subdivision was devised (Section 5.2) in which amphibole compositional space was subdivided into nine regions in which each of the 'end members' were respectively the dominant component of the basic atomic formulae plotting within the region. These were termed sensu dominante regions, see Fig 5.6 and Table 5.1. It is suggested that the concept of the dominant component is intrinsically more valuable than a nomenclature based on previous usage(cf Miyashiro 1957, Leake 1968) or a number of cubic cells (cf Whittaker 1968). Sensu dominante nomenclature was used extensively in Chapters 7 and 8.

It is sometimes advantageous to be able to describe a basic atomic formula as a linear combination of 'end member' components. Because there are more than four vertices in three dimensional amphibole compositional space it is possible to derive alternative equivalent combinations for other than 'end members' themselves. It was suggested (Section 5.3) that where such a combination is required the 'end member' combination with the maximum proportion of the sensu dominante component present should normally be used or where this is not unique that with the smaller number of components. To achieve this Table 5.2 of equivalent 'end member' combinations was given. Table 5.2 can also be used to maximise other than the sensu dominante component as for example when considering amphiboles near a binary join between 'end members'. In deriving the sensu dominante nomenclature the Na^{+}, Mg^{2+}, Al^{3+} substituted 'end members' of Phillips & Layton (1964) and Phillips (1966) were retained. Two of these, miyashiroite and sundiusite have been discredited as amphibole names (Fleischer 1965; 1966) since neither had been synthesised or reported

as the dominant component of any natural amphibole. A search of the amphibole data file located 6 amphiboles in M sensu dominante, of which 5 were in M sensu extenso and 115 amphiboles in Su sensu dominante of which 15 were in Su sensu extenso (Section 5.4). While most showed various degrees of ferrous, ferric iron substitution for Mg^{2+} and Al^{vi} it was suggested that because basic atomic formulae of natural amphiboles did occur with $NaCaNaMg_3Al_2Si_6Al_2O_{22}(OH)_2$ and $NaNa_2Mg_3Al_2Si_7Al\ O_{22}(OH)_2$ as the dominant component and in excess of 50 per cent there were strong grounds for retaining sundiusite and miyashiroite as 'end member' names. This is similar to the present use of tschermakite and allows all the 'end members' to be named after Na^+, Mg^{2+}, Al^{3+} substituted amphiboles.

Since the nomenclature of amphibole compositional space was based entirely on Na^+, Mg^{2+}, Al^{3+} 'end members', it is possible to indicate the extent of geologicaly important substitutions such as Fe^{2+} for Mg^{2+} and Fe^{3+} for Al^{vi} in a consistent manner by qualifying the sensu dominante name with appropriate adjectival prefixes (Section 5.5). Thus two amphiboles with $Mg^{2+} > Fe^{2+}$, $Fe^{3+} > Al^{vi}$ and $Fe^{2+} > Mg^{2+}$ $Fe^{3+} > Al^{vi}$ both with Pa as the dominant component of the basic atomic formula would be termed ferri Pa sensu dominante and ferro ferri Pa sensu dominante respectively. A similar approach can be applied to other substituting ions provided the role of the substituting ion is known. The titaniferous amphiboles were considered separately in Section 5.5.1. All the apparently reliable analyses with $Ti^{4+} \geqslant 0.5$ atoms and H_2O^+, F or Cl determined and almost all those with $Ti^{4+} \geqslant 0.5$ in the amphibole data file were found to be similar with $Al^Z > 1.5$, $Al^Y > 1.0$, $Na^X < 0.5$, $Na^A > 0.5$ (Ca + Na > 1.33). In view of this it was considered appropriate to use kaersutite for such analyses in addition to their sensu dominante nomenclature.

In order to distinguish basic atomic formulae of the calcic amphiboles from those with Mg^{2+}, Fe^{2+} or Mn^{2+} in the X group an extended form of the basic atomic formula was devised (Section 5.6). This had four independant variables (Al^{Z}, Al^{Y} Na^{X}, Ca or Mg^{X}) and a further six extreme basic atomic formulae were possible. Three of these were found to correspond to previously named amphiboles, anthophyllite, gedrite, magnesio-richterite and a fourth one ($Na\ Mg_2Mg_4\ Al\ Si_6Al\ O_{22}(OH)_2$) was named soda-gedrite after it was found that natural amphiboles occurred with greater than 50 per cent of the component present. The most successful three dimensional representation involving three out of the four variables of the extended basic atomic formula was termed extended amphibole compositional space (Fig 5.10). Since only three variables were used individual points represent more than one basic atomic formula and while the 'end members' of amphibole compositional space and the additional six extreme compositions do not all correspond to vertices of the space. Because of this no attempt was made to subdivide the space into <u>sensu dominante</u> regions. From the observed distribution of basic atomic formulae in extended amphibole compositional space (Chapter 7) a three fold subdivision at Mg^{X} 0.66 ($Ca + Na^{X}$ 1.33), Mg^{X} 1.33 ($Ca + Na^{X}$ 0.66) appeared appropriate. Amphiboles with Mg^{X} in excess of 1.33 were termed FeMgMn amphiboles, those with Mg^{X} less than 0.66 were further subdivided at Na^{X} 0.66 and 1.33. These three subdivisions and the corresponding three of amphibole compositional space were termed in order of increasing Na^{X} the calcic, soda calcic and alkali amphiboles. The remaining zone of extended amphibole compositional space with Mg^{X} 0.66 - 1.33 was unnamed. It was suggested that <u>sensu dominante</u> nomenclature could be extended to calcic, soda calcic and alkali amphiboles, that is those with Mg^{X} up to 0.66 atoms.

Two axis plots of views of both amphibole compositional space

and extended amphibole compositional space were used to show the general distribution of natural amphiboles (Chapter 7) and the relationship between amphibole composition and host rock type (Chapter 8).

9.5. Distribution of basic atomic formulae.

The distribution of basic atomic formulae over amphibole and extended amphibole compositional space was illustrated in Chapter 7 (Figs 7.1 - 7.28). Despite the diverse modes of occurrence and large number of analyses used it was found that balanced basic atomic formulae of natural amphiboles plotted predominantly in either the calcic, alkali or FeMgMn groups and were less common and almost completely absent in the soda calcic and unnamed amphibole groups respectively. The observed distribution is consistent with what is known of miscibility relations between the FeMgMn - calcic and FeMgMn - alkali amphiboles from experimental evidence (Cameron 1971) and exsolution phenomena in naturally occurring amphiboles (Ross, Papike & Shaw 1969, Robinson et al. 1971). A number of workers (Sundius 1946; Boyd 1959; Ernst 1968) have attributed the relative infrequency of soda calcic amphiboles to a miscibility gap. As far as the author is aware reports of exsolution textures in which both host and exsolved phases were either calcic, soda calcic or alkali amphiboles have not been confirmed, (see Section 7.2), however pairs of calcic or alkali and less commonly soda calcic amphiboles in apparent textural and chemical equilibrium have been reported from a small number of localities, (see Section 7.2.2).

Comparison of the distribution of basic atomic formulae of such pairs contained in the amphibole data file with the distribution of basic atomic formulae (cf Figs 7.1, 7.2, 7.4, 7.5, 7.25, 7.26 with 7.30 - 7.33) showed that with the exception of those pairs from the

Sanbagawa Metamorphic Belt (Fig 7.32) the separation corresponded to the limits of the soda calcic amphiboles. Further with the exceptions above the apparently coexisting pairs had either Tr, G or Pa but not R or Su as the dominant components of the basic atomic formulae and their tie lines did not extend towards richterite or to high Al^Z values. In contrast inspection of the low Al^Z soda calcic amphiboles showed that the majority were from igneous or hydrothermal parageneses, typically with R as the dominant component, and lay on the richterite side of the tie lines. The metamorphic amphiboles on the other hand were much less numerous but included only twelve analyse in the fields of Tr, Ts, Su and G s.d. which could be considered intermediate between at least some of the pairs and in addition two R s.d. The combination of evidence from the relative infrequency of soda calcic compared with calcic and alkali amphiboles, the existence of calcic - alkali amphibole pairs in apparent equilibrium and the presence of only 12 out of 2650 analyses which are intermediate was considered consistent with, although not proof of, a solvus between the calcic and alkali amphiboles. The location of the proposed solvus lies between Tr - G and Pa - G but there was no evidence for its extension towards richterite or sundiusite. Tentative facies assignments for the pairs suggested conditions of formation intermediate between those of the greenschist and glaucophane lawsonite schist facies or the high temperature blueschist facies while there was some evidence that under the conditions of the Sanbagawa Metamorphic Belt the solvus was either reduced or absent. It is apparent therefore that there is a need for experimental work to be undertaken in the join Tr - G to provide evidence regarding the existence of the postulated solvus and to determine the pressure and temperature over which this may exist. Such information would be potentially valuable in interpretating the physical conditions metamorphic rocks intermediate between the greenschist, glaucophane lawsonite schist, and

high temperature blueschist facies formed under.

A hiatus in the Al^Z of the calcic amphiboles and the existence of 'actinolite' - 'hornblende' pairs has been interpretated by a number of workers as evidence of a solvus within the calcic amphiboles, (Section 7.2.1). A bimodal distribution of Al^Z in calcic amphiboles was observed (Fig. 7.29) with maxima at 0.0 - 0.1 and 1.6 - 1.7 and a minimum at 0.4 - 0.5, while a search of the amphibole data file located only one apparently coexisting pair with values for Al^Z which straddled the observed minimum,(Fig 7.21). However, it was suggested that since there was only a single pair and only calcic amphiboles from calcareous host rocks showed a bimodal distribution of Al^Z (Fig. 7.29) that the solvus, if it existed must be restricted. Jasmund & Schafer (1972) and Ernst (1972) failed to find evidence for a solvus in an experimental study of the join Tr - Ts and in natural amphiboles from the Sanbagawa Metamorphic Belt respectively. It was concluded tentatively that evidence for a solvus was inconclusive.

9.6. General features of basic atomic formulae of amphiboles from various igneous and metamorphic parageneses.

Using the original authors name for the host rock as contained in relation OCCURRENCE (Chapter 4, Appendix 9) the distribution of basic atomic formulae in amphibole compositional space and extended amphibole compositional space, the extent of $Mg^{2+} - Fe^{2+}$, $Al^{vi} - Fe^{3+}$ substitution in the atomic formulae, and the nomenclature of amphiboles in a number of igneous (Section 8.1) and metamorphic (Section 8.2) host rock categories were described for amphiboles in the amphibole data file with balanced basic atomic formulae and either H_2O, F or Cl determined. Despite the limitations imposed by using the original authors nomenclature and the impracticality, in most instances, of separating amphiboles in equilibrium from those which were not in equilibrium, it was found that the distribution and nomenclature of

amphiboles from individual host rock categories was distinctive.

Perhaps the most striking distinctions were between amphiboles from igneous and those from metamorphic host rock categories (for definitions of these categories see Section 7.1). Igneous amphiboles in Ed s.d. and the FeMgMn amphiboles were found to be uncommon compared with amphiboles from metamorphic rocks. The reverse situation applied to R, Ec s.d. and kaersutite. The possibility that these distinctions could be attributed, at least in part, to bias in sampling was not ruled out altogether. However, searches of the entire amphibole data file and the previous recognition of some of the distinctive features tended to reduce this possibility. The observed distributions and where appropriate published experimental data on amphibole stability were used to support tentative suggestions as to the more important factors controlling specific distributions.

Only three FeMgMn amphiboles from igneous host rocks were illustrated in Figs 7.1 - 7.28. They were all cummingtonite - grunerite. The apparent scarcity of such amphiboles in igneous rocks was attributed (Section 8.3.1) to the relatively low thermal stability of cummingtonite - grunerite (Schurmann 1968). This is consistent with the observed occurrence of cummingtonite - grunerite as a secondary mineral after orthopyroxene, as a late stage reaction product of olivine and quartz and as low temperature phenocrysts in acid extrusives. The absence of gedrite but not anthophyllite may be explained in a similar manner. Additional factors such as magma composition, in particular the presence of Ca^{2+}, may have an important bearing on the relative scarcity of igneous FeMgMn amphiboles.

The complete lack of edenitic amphiboles from igneous host rocks and the scarcity of Ed s.d. from such paragenese was attributed (Section 8.3.2) to a postulated low thermal stability of edenite and ferroedenite. This suggestion is speculative since, as far as the

writer is aware, the stability of edenite and ferroedenite have not been determined experimentally.

Kaersutites (as defined in Section 5.5.1) were found (Section 8.3.3) to be almost exclusively confined to igneous host rocks, in particular silica undersaturated, often alkali rich feldspathoidal parageneses. Only a single metamorphic kaersutite, from an eclogite, was found in the illustrated analyses (Table 8.1). Examination of the entire amphibole data file located a number of further apparently reliable analyses from eclogites but none form other metamorphic host rocks. It was not possible to define the factors necessary for the crystallisation of kaersutite. However, the apparently complete absence from metamorphic rocks formed under normal regional and contact metamorphic facies regimes and the association of the eclogite kaersutites with igneous rocks suggested that somewhat extreme conditions not normally found during metamorphism were required for kaersutite to crystallise in natural assemblages.

In contrast amphiboles with R or Ec as the dominant component of the basic atomic formula were found to be fairly common in igneous and calcareous host rocks, but absent, or at least extremely rare in the remaining metamorphic host categories (Section 8.3.4). Following Phillips & Rowbotham (1968) this feature of their distribution was attributed to the peculiar chemical requirements of both amphiboles although the presence of a solvus in the vicinity of richterite may also be significant.

Igneous rocks were subdivided into six categories, ultramafic - ultrabasic, basic, intermediate, acid, basic alkali, and alkali. The distribution of basic atomic formulae, variation in nomenclature and extent of Mg^{2+}-Fe^{2+}, Al^{vi} - Fe^{3+} substitution were found to show gradational changes between the categories. In passing from ultrabasic - ultramafic, through basic and intermediate to acid host

rocks a gradual decrease in the lower limit of Al^{vi} (increase in Si^{4+}) was found for calcic amphiboles. This was attributed to the availability of silica in the magma rather than due to the temperature of crystallisation (cf Harry 1950; Leake 1971), since the calcic amphiboles of the basic alkali and alkali host rocks also showed high Al^{iv} (low Si^{4+}) contents. As in the other mafic silicates the amphiboles showed the substitution of Mg^{2+} by Fe^{2+} in passing from ultramafic - ultrabasic to acid and basic alkali to alkali host rocks. Aluminium was reduced and substituted by ferric iron probably in response to decreasing Al^{3+} availability and increasing water and hence iron oxidation state in the magma.

Since it was not possible to subdivide metamorphic amphiboles in terms of facies and host rock composition very little could be inferred regarding the variation of amphibole composition with metamorphic grade. However, amphiboles from eclogites were found (Section 8.3.6) to be more varied than might be expected from a rock type which has been given metamorphic facies status. While some of the variation may be attributed to retrogression the recognition by Coleman et al. (1965) that garnet and to a lesser extent pyroxene composition varied systematically with the mode of occurrence of eclogite prompted a closer examination of the variation exhibited by the amphiboles.

Amphiboles from rocks complying to a non-genetic definition of eclogite were separated from the amphibole data file. Four modes of occurrence were recognised, (i) inclusions in kimberlite and ultrabasic bodies, (ii) associated with rocks belonging to the amphibolite and granulite facies, (iii) associated with rocks belonging to the albite epidote amphibolite facies, and (iv) associated with glaucophane bearing schists. Plots of Al^{Z} versus Na^{X} for the calcic, soda calcic and alkali amphiboles and Al^{Z} verus Al^{Y} for the calcic amphiboles (Fig 8.8) showed that primary amphiboles from plagioclase

free assemblages were not only varied in composition but the composition varied systematically with the mode of occurrence. Secondary amphiboles displayed a less well defined distribution. It was suggested (Section 8.3.6) that the large and systematic variation exhibited by the basic atomic formulae of primary amphiboles from eclogites in terms of their mode of occurrence coupled with the relationship reported for the garnets and pyroxenes (Coleman et al. 1965) was consistent with eclogites having formed over a range of temperatures and pressures. The composition of primary amphibole may prove to be an important diagnostic feature of the mode of occurrence of eclogite.

9.6. Concluding remarks.

This work has demonstrated the feasibility of using a large collection of analyses and a number of graphical representations based on the simplifying concept of the basic atomic formula to summarise in a convenient way the chemical variation exhibited by natural amphiboles. The ability to summarise what is probably a significant proportion of the published chemical analyses of amphiboles has led to a clearer understanding of the oustanding problems of amphibole mineralogy. The existence of solvi within the amphibole group were confirmed and inferred from the non-random distribution of analyses within amphibole compositional space and extended amphibole compositional space. By outlining the variation exhibited by the amphiboles from a number of host rock categories it was possible to make tentative suggestions as to the factors controlling amphibole composition in specific environments. Further, using the observed distribution it was possible to focus attention both on those compositions which appear commonly and those which are uncommon in specific host rocks and to relate additional analyses to a body of information concerning amphiboles from similar rock types or amphiboles of similar composition.

REFERENCES

Adams, F. D. (1903) The Monteregian Hills, Canadian petrographical province. J. Geol., 11, 259-282.

Addison, W. E., & White, A. D. (1968) Spectroscopic evidence for the siting of lithium ions in riebeckite. Mineral. Mag., 36, 743-745.

Agrell, S. O., Scoon, J. H., Muir, I. D., Long, J. V. P., McConnell, J. D. C., & Peckett, A. (1970) Observations on the chemistry, mineralogy and petrology of some Apollo 11 lunar samples. Proc. Apollo 11 Sci. Conf. (Suppl. to Geochim. Cosmochim. Acta 34), 1, 93-128.

Ainberg, L. F. (1930) In: Forts. Mineralogie Krist. Petrologie, (1935), 19, 271.

Albee, A. L., & Chodos, A. A. (1970) Semiquantitative electron microprobe determination of Fe^{2+}/Fe^{3+} and Mn^{2+}/Mn^{3+} in oxides and silicates and its application to petrologic problems. Am. Miner., 55, 491-501.

Alderman, A. R. (1936) Eclogites from the neighbourhood of Glenelg, Inverness-shire. Q. Jl. geol. Soc. Lond., 92, 488-530.

Andreev, Yu. K. (1957) A new variety of alkali-amphibole - magnesio-arfvedsonite. Trans. Inst. Geol. of Ore-deposits Petr. Min. & Geochem., 10, 12-50.

Annersten, H., & Ekström, T. (1971) Distribution of major and minor elements in coexisting minerals from a metamorphosed iron formation. Lithos, 4, 185-204.

Aoki, K. (1963) The kaersutites and oxykaersutites from alkalic rocks of Japan and surrounding areas. J. Petrology, 4, 198-210.

———, (1970) Petrology of kaersutite - bearing ultramafic and mafic inclusions in Iki Island, Japan. Contr. Mineral. and Petrology, 25, 270-283.

Bancroft, G. M., & Burns, R. G. (1969) Mössbauer and absorption spectral study of alkali amphiboles. Mineral. Soc. Amer. Spec. Pap., 2, 137-148.

———, ———, & Maddock, A. G. (1967a) Determination of cation distribution in the Cummingtonite - Grunerite series by Mössbauer spectra. Am. Miner., 52, 1009-1026.

———, ———, ———, (1967b) Application of the Mössbauer effect to silicate mineralogy - I Iron silicates of known crystal structure. Geochim. Cosmochim. Acta, 31, 2219-2246.

———, ———, ———, & Strens, R. G. (1966) Cation distribution in anthophyllite from Mössbauer and infrared spectroscopy. Nature, 212, 913-915.

———, ———, & Stone, A. J. (1968) Application of the Mössbauer effect to silicate mineralogy - II. Iron silicates of unknown and complex crystal structures. Geochim. Cosmochim. Acta, 32, 547-559.

Bancroft, J. A., & Howard, W. V. (1923) The essexites of Mount Royal, Montreal, P. Q. Trans. Roy, Soc. Canada, 17, 13-43.

Banno, S (1964) Petrologic studies on Sanbagawa crystalline schists in the Bessi-ino district, central Sikoku, Japan. J. Fac. Sci. Tokyo Univ., 15, 203-319.

Bauer, L. H., & Berman, H. (1930) Notes on some Franklin minerals. Am. Miner., 15, 340-348.

Bearth, P. (1959) Ueber Eklogite, Glaucophanscheifer und metamorphe Pillowlaven. Schweiz. miner. petrogr. Mitt., 39, 267-286.

Best, M. G. (1970) Kaersutite - peridotite inclusions and kindred megacrysts in basanitic lavas, Grand Canyon, Arizona. Contr. Mineral. and Petrology, 27, 25-44.

Binns, R. A. (1967) Barroisite - bearing eclogite from Naustdal, Sogn og Fjordane, Norway. J. Petrology, 8, 349-371.

————, (1969) High - pressure megacrysts in basanitic lavas near Armidale, New South Wales, Am. J. Sci., 267A, 33-49.

Bloss, F. D. (1966) An Introduction to the Methods of Optical Crystallography. Holt, Rinehart and Winston, New York, 294pp.

Bloxam, T. W., & Allen, J. B. (1960) Glaucophane - schist, eclogite, and associated rocks from Knockmoral in the Girvan - Ballantrae Complex, South Ayrshire. Trans. Roy. Soc. Edinburgh, 64, 1-28.

Blyth, F. G. H., & Lambert, R. St. J. (1970) Chemical data from the Malvernian of the Malvern Hills, Herefordshire. Q. Jl. geol. Soc. Lond., 125, 543-555.

Bonnischen, B. (1969) Metamorphic pyroxenes and amphiboles in the Biwabik iron formation, Dunka river area, Minnesota. Mineral. Soc. Amer. Spec. Pap., 2, 217-239.

Borg, I. Y. (1956) Glaucophane schists and eclogites near Healdsburg, California. Bull. Geol. Soc. Amer., 67, 1563-1584.

————, (1967a) On conventional calculation of amphibole formulae from chemical analyses with inaccurate $H_2O(+)$ and F determinations. Mineral. Mag., 36, 583-590.

————, (1967b) Optical properties and cell parameters in the glaucophane - riebeckite series. Contr. Mineral. and Petrology, 15, 67-92.

Borley, G. D., Suddaby, P., & Scott, P. (1971) Some xenoliths from the alkalic rocks of Teneriffe, Canary Islands. Contr. Mineral. and Petrology, 31, 102-114.

Bornoman-Starynkevich, I. D. (1960) The chemical formula of minerals. IV. Amphiboles. Mem. All Union Min. Soc., 89, 236-247.

Bose, M. K. (1963) Calciferous brown amphibole in alkali gabbro of Koraput, Orissa, India. Am. Miner., 48, 1405-1409.

Bowen, N. L., & Schairer, J. F. (1935) Grünerite from Rockport Massachusetts and a series of synthetic fluor amphiboles.

Am. Miner., 20, 543-551.

Bown, M. G. (1965) A new amphibole polymorph in intergrowth with tremolite: clino-anthophyllite ?. (abstr.). Am. Miner., 51, 259-260.

Boyd, F. R. (1959) Hydrothermal investigation of amphiboles. In: P. H. Abelsen, ed., Researches in Geochemistry. New York. 377-396.

Brady, J. B. (1974) Coexisting actinolite and hornblende from West - central New Hampshire. Am. Miner., 59, 529-535.

Brock, P. W. G., Gellatty, D. C. , & Knorring, O. von. (1964) Mboziite, a new sodic amphibole end - member. Mineral. Mag., 33, 1057-1064.

Brothers, R. N. (1954) Glaucophane schists from the North Berkeley Hills, California. Am. J. Sci., 252, 614-626.

Bryhini, I., & Griffin, W. L. (1971) Zoning in eclogite garnets from Nordfjord, West Norway. Contr. Mineral. and Petrology, 32, 112-125.

Buckley, A. N., & Wilkins, R. W. T. (1971) Mössbauer and infrared study of a volcanic amphibole. Am. Miner., 56, 90-100.

Buerger, M. J. (1927) Optical notes on some of the variable contact minerals from Edenville, New York. Am. Miner., 12, 374-378.

Burns, R. G. (1965) Electronic spectra of silicate minerals: Applications of crystal - field theory to aspects of geochemistry. Ph. D. thesis, Univ. of Calif., Berkeley, California.

————————, (1970) Mineralogical Applications of Crystal Field Theory. Cambridge Univ. Press. 224pp.

————————, & Greaves, C. J. (1971) Correlation of infrared and Mössbauer site population measurements of actinolites. Am. Miner., 56, 2010-2033.

————————, & Law, A. D. (1970) Hydroxyl stretching frequencies in the infrared spectra of anthophyllites and gedrites. Nature, 226, 73-75.

———————, & Prentice, F. J. (1960) Distribution of iron cations in the crocidolite structure. Am. Miner., 53, 770-776.

———————, & Strens, R. G. J. (1966) Infrared study of the hydroxyl bands in clinoamphiboles. Science, 153, 890-892.

Butler, P. Jr (1969) Mineral compositions and equilibria in the metamorphosed iron formations of the Gagnon region, Quebec, Canada. J. Petrology, 16, 56-100.

Callegari, E., & Monese, A. (1961) Studio petrogenetico dei bordi di reazione metamorfico-metasomatici attorno a lenti ultrafemiche incluse nel granito di S. Fedelino (Sondrio). Rend. Soc. Min. Ital., 17, 147-192.

Cameron, M. L. (1971) Amphibole phase relations along the join $Mg_{3.5}Fe_{3.5}Si_8O_{22}(OH)_2$ - $Ca_2Mg_{2.5}Fe_{2.5}Si_8O_{22}(OH)_2$. Carnegie Inst. Year Book, 70, 145-150.

Cameron, M., & Gibbs, G.V. (1971) Refinement of the crystal structure of two synthetic fluor- richterites. Carnegie Inst. Year Book, 70, 150-153.

Campbell, I., & Schenk, E. T. (1950) Camptonite dykes near Boulder Dam, Arizona. Am. Miner., 35, 671-692.

Carmichael, I. S. E. (1967a) The iron-titanium oxides of some salic volcanic rocks and their associated ferromagnesian silicates. Contr. Mineral. and Petrology, 14, 36-64.

———————, (1967b) The mineralogy and petrology of the volcanic rocks from the Leucite Hills, Wyoming. Contr. Mineral. and Petrology, 15, 24-66.

Chamberlain, D. D., & Boyce, R. F. (1974) SEQUEL: A structured English query language. ACM-SIGFIDET Workshop on data description access and control. 16pp.

Charles, R. W. (1972) Phase equilibria of the richterite end members $NaCa_2Mg_5Si_8O_{22}(OH)_2$ and $NaCa_2Fe_5Si_8O_{22}(OH)_2$. Carnegie Inst. Year Book, 71, 506-510.

Chayes, F. (1972) Rock information system - version III. Washington D.C.

Chesnokov, B. V. (1960) Rutile bearing eclogites from the Shibino Village deposit in the Southern Urals. Intern. Geology Rev., 2, 936-945.

Codd, E. F. (1970) A relational model of data for large shared data banks. Comm ACM., 13, 377-387.

————, (1971) Normalised data base structure: A brief tutorial. Proc. ACM-SIGFIDET Workshop on Data Description, Access and Control, San Diego.

Coleman, R. G., Lee, D. E., Beatty, L. B., & Brannock, W. W. (1965) Eclogites and eclogites: their differences and similarities. Bull. Geol. Soc. Amer., 76, 483-508.

Colville, A. A., & Gibbs, G. V. (1964) Refinement of the crystal structure of riebeckite (abstr). Geol. Soc. Amer. Spec. Paper, 82, 31.

Colville, P. A., Ernst, W. G., & Gilbert, M. C. (1966) Relationship between cell parameters and chemical composition of monoclinic amphiboles. Am. Miner., 51, 1727-1754.

Conquere, F. (1971) Les pyroxénolites à amphibole et les amphibolites associées aux lherzolites du gisement de Lherz (Ariège, France): un example du rôle de l'eau au cours de la crystallisation fractionnée des liquides issus de la fussion partielle de lherzolites. Contr. Mineral. and Petrology, 33, 32-61.

Cooper, A. F. (1972) Progressive metamorphism of metabasic rocks from the Haast Schist Group of Southern New Zealand. J. Petrology, 13, 457-492.

————, & Lovering, J. F. (1970) Greenschist amphiboles from Haast River, New Zealand. Contr. Mineral. and Petrology, 27, 11-24.

Couyat, A. (1908) In: Leake, B. E. (1968) A catalog of

analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Daniels, J. L. (1956) The metamorphic petrology of the Pre-Cambrian rocks of northern Baffin Island. Ph.D. Thesis, Univ. Manchester.

Deer, W. A. (1935) The Cairnsmore of Carsphairn igneous complex. Q. Jl. Geol. Soc. Lond., 91, 47-76.

_____, Howie, R. A., & Zussman, J. (1963) Rock Forming Minerals. Vol. 2, Longman, London, 379pp.

Dickey, J. S. Jr (1968) Eclogites and other inclusions in the mineral breccia member of the Deborah volcanic formation at Kakanui, New Zealand. Am. Miner., 53, 1304-1319.

Dixon, C. J. (1970) Machine languages for representation of Geological information. Systematics Assoc. Spec. Vol. No. 3. 'Data Processing in Biology and Geology', ed Cutbill, J. L. 123-134.

Dodge, E. C. W., Ross, D. C. (1971) Coexisting hornblendes and biotites from granitic rocks near the San Andreas fault, California. J. Geol., 79, 155-172.

Douglas, J. A. V., & Plant, A. G. (1968) Amphibole: First occurrence in an enstatite chondrite (abstr). 31st Ann. Meeting Meteoritical Soc. Cambridge, Mass.

Dowty, E., & Clark, J. R. (1973) Crystal structure refinement and optical properties of a Ti^{3+} fassaite from the Allende meteorite. Am. Miner., 58, 230-242.

Drysdall, A. R., & Newton, A. R. (1960) Blue asbestos from Lusaka, Northern Rhodesia, and its bearing on the genesis and classification of this type of asbestos. Am. Miner., 45, 53-59.

Dunitz, J. D., & Orgel, L.E. (1957) Electronic properties of transition element oxides II. Cation distribution amongst

octahedral and tetrahedral sites. J. Phys. Chem. Solids, 3, 318-333.

Du Rietz, T. (1935) Peridoitäes, serpentinites, and soapstones of northern Sweden, with special reference to some occurrences in northern Jamtland. Geol. För. Förh. Stockholm, 57, 133-260.

Edwards, A. B. (1938) The tertiary volcanic rocks of central Victoria. Q. Jl. geol. Soc. Lond., 94, 243-318.

Eitel, W. (1922) Die Mischkristallbildung in der Gruppe der alkali - und tonerdhaltigen Hornblenden, dargestellt in den Vierstoffsystem SiO_2-CaO-(MgFe)O-$(AlFe)_2O_3$ und RC-SiO_2-R_2O_3-R_2O. Neues. Jahrb. Min., 47, 201-253.

Erdsmannsdorffer, O. H. (1929) Uber Alkalihornblenden aus dem Radautal, Sitzungsber. Heidelberg Akad. Wiss. Math. naturw. Kl., 17, 6pp.

Erlank, A. J., & Finger, L. W. (1970) The occurrence of potassic richterite in a mica nodule from the Wesselton kimberlite, South Africa. Carnegie Inst. Year Book, 68, 320-324.

Ernst, W. G. (1961) Stability relations of glaucophane. Am. J. Sci., 259, 735-765.

———, (1963)Petrogenesis of glaucophane schists. J. Petrology, 4, 1-30.

———, (1964) Petrochemical study of coexisting minerals from low grade schists, eastern Shikoku, Japan. Geochim. Cosmochim. Acta, 28, 1631-1668.

———, (1968) Amphiboles. Springer-Verlag, New York, 125pp.

———, (1972) Ca-amphibole paragenesis in the Shirataki district, Central Shikoku, Japan. 73-94. In: Studies in mineralogy and Precambrian geology. The John W. Gruner volume eds. Doe, B. R., Smith, D. K., Geol. Soc Amer. Mem., 135.

———, Seki, Y., Onuki, H., & Gilbert, M. C. (1970) Comparitive study of low-grade metamorphism in the California Coast Ranges and the Outer Metamorphic Belt of Japan. Geol.

Soc. Amer. Mem., 124, 276pp.

_____, & Wai, C. M. (1970) Mössbauer, infrared, X-ray and optical study of cation ordering and dehydrogenation in natural and heat treated sodic amphiboles. Am. Miner., 55, 1226-1258.

Eskola, P. (1914) On the petrology of the Orijarvi Region in southwestern Finland. Bull. comm geol. Finl., 40, 277pp.

_____, (1921) On the eclogites of Norway. Vidensk-selskapets Skr. Kristiana, 1, Matematisk-Naturvidenskapelig. Kl., 8, 1-118.

Ewart, A., Green, D. C., Carmichael, I. S. E., & Brown, F. H. (1971) Voluminous low temperature rhyolitic magmas in New Zealand. Contr. Mineral. and Petrology, 33, 128-144.

_____, Hildreth, W., & Carmichael, I. S. E. (1975) Quarternary acid magmas in New Zealand. Contr. Mineral. and Petrology, 51, 1-27.

Fabries, M. J. (1963) D.Sc. Thesis. Univ. of Nancy, France.

_____, (1966) Une représentation graphique des principales substitutions recontrées les amphiboles calciques et sodiques. Compt. Rend. Acad. Sci. Paris, 262, Ser. D, 1824-1827.

Fedoseev, A. D., Grigoreva, L. F., Chigareva, O. G., & Romanov, D. P. (1970) Synthetic fibrous fluoramphiboles and their products. Am. Miner., 55, 854-863.

Felix, R. (1970) Register of amphiboles. Unpublished document submitted to the I.M.A. Commission on New Minerals and Mineral Names (Amphibole Group).

Finger, L.W. (1969) The crystal structure and cation distribution of a grunerite. Mineral Soc. Amer. Spec. Paper, 2, 95-100.

_____, (1970a) The structure refinement and cation distribution of an anthophyllite. Am. Miner., 55, 300 .

_____, (1970b) Refinement of the crystal structure of an anthophyllite. Carnegie Inst. Year Book, 68, 283-288.

———————, & Chashi, Y. (1974) Preliminary results of the refinement of the crystal structure of holmquistite. Carnegie Inst. Year Book, 73, 535-539.

———————, & Zoltai, T. (1967) Cation distribution in grunerite (abstr). Trans. Amer. Geophys. Union, 48, 233-234.

Fischer, K.-F. (1966) A further refinement of the crystal structure of cummingtonite $(Mg,Fe)_7Si_8O_{22}(OH)_2$. Am. Miner., 51, 814-818.

Fleischer, M. (1965) New mineral names. Am. Miner., 50, 1507.

———————, (1966) Index of new mineral names, discredited minerals, and changes of mineralogical nomenclature in volumes 1-50 of the American Mineralogist. Am. Miner., 51, 1248-1357.

Forbes, W. C. (1971) Synthesis and stability relations of richterite $NaCa_2Mg_5Si_8O_{22}(OH)_2$. Am. Miner., 56, 997-1004.

Foshag, W. F. (1936) Canophyllite and zincian amphibole from Franklin Furnace, New Jersey. Am. Miner., 21, 63-67.

Frisch, T. (1970) Chemical variation among the amphiboles of Shefford Mountain a Monteregian intrusion in southern Quebec. Can. Mineral., 10, 553-570.

Ghose, S. (1961) The crystal structure of cummingtonite. Acta Crystallogr., 14, 622-627.

———————, (1965) A scheme of cation distribution in the amphiboles. Mineral. Mag., 35, 46-54.

———————, & Hellner, E. (1959) The crystal structure of grunerite and observations on the Mg-Fe distribution. J. Geol., 67, 691-701.

———————, & Weidner, J. R. (1972) Mg^{2+}-Fe^{2+} order-disorder in cummingtonite, $(Mg,Fe)_7Si_8O_{22}(OH)_2$: A new geothermometer. Earth Planetary Sci. Letts., 16, 346-354.

Gibbs, G. V. (1966) In: Short Course Lecture Notes: Chain Silicates. American Geological Institution.

———————, (1969) Crystal structure of protoamphibole. Mineral. Soc. Amer. Spec. Paper, 2, 101-109.

———————, Bloss, F. D., & Shell, H. R. (1960) Proto-amphibole a new polytype, Am. Miner., 45, 974-989.

———————, Miller, J. L., & Shell, H. R. (1962) Synthetic fluor - magnesio - richterite. Am. Miner., 47, 75-82.

Gier, T. E., Cox, H. L., & Young, H. S. (1964) The hydrothermal synthesis of sodium amphiboles. Inorganic Chem., 3, 1001-1004.

Gilbert, M. C. (1966) Synthesis and stability of the hornblende-ferropargasite series. Am. J. Sci., 264, 698-742.

Ginzburg, I. V. (1965) Holmquistite and its structural variant clinoholmquistite. Trudy Mineralog. Muzeya Akad. Nauk. SSSR., 16, 73-89.

Graham, C. M. (1974) Metabasite amphiboles of the Scottish Dalradian. Contr. Mineral. and Petrology, 47, 165-185.

Greaves, C. R., Burns, R. G., & Bancroft, G. M. (1971) Resolution of actinolite Mössbauer spectra into three ferrous doublets. Nature Physical Science, 229, 60-61.

Green, D. H. (1967) An experimental investigation of the gabbro to eclogite transformation and its petrological implications. Geochim. Cosmochim. Acta, 31, 767-833.

Greenwood, H. J. (1963) The synthesis and stability of anthophyllite. J. Petrology, 4, 317-351.

Gunn, B. M. (1972) The fractionation of kaersutite in basaltic magmas. Can. Mineral., 11, 840-850.

Hafner, S. S., & Ghose, S. (1971) Iron and magnesium distribution in cummingtonites $(Fe, Mg)_7Si_8O_{22}(OH)_2$. Z. Kristallogr., 133, 301-326.

Hallimond, A. F. (1943) On the graphical representation of the calciferous amphiboles. Am. Miner., 28, 65-89.

Harker, R. I. (1963) The older ortho-gneiss of Carn Chuinneag and Inchbae. J. Petrology, 3, 215-237.

Harrington, B. J. (1903) On the composition of some Canadian amphiboles. Am. J. Sci., 15, 392-394.

Harrison, R. K., & Sabine, P. A. (1970) A petrological - mineralogical code for computer use. Inst. Geol. Sci. Rep. No. 70/6, 134pp.

Harry, W. T. (1950) Aluminium replacing silicon in some silicate lattices. Mineral. Mag., 29, 142-149.

Hartman, P. (1969) Can Ti^{4+} replace Si^{4+} in silicates ?. Mineral. Mag., 37, 366-369.

Harumoto, A. (1933) On the kaersutite and the pigeonite in the volcanic ejecta, Utsurya Island. Chikyu (The Globe), 19, 96-110.

Hauy, C. (1801) Traité de Minéralogie. Paris.

Hawthorne, F. C., & Grundy, H. D. (1973a) The crystal chemistry of the amphiboles. I: Refinement of the crystal structure of ferrotschermakite. Mineral. Mag., 39, 36-48.

———————, ———————, (1973b) The crystal chemistry of the amphiboles. II: Refinement of the crystal structure of oxy-kaersutite. Mineral. Mag., 39, 390-400.

———————, ———————, (1973c) The crystal structure and site chemistry of a zinc manganese cummingtonite by a least squares refinement of X-ray and Mössbauer data. Am. Miner., 58, 1103.

Henry, N. F. M. In: Leake, B. E. (1968) A catalog of analysed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Heritsch, H., & Kahler, E. (1960) Struckturunterschung an zwei Kluftkarinthinen, Ein Beitrag zur Karinthinfrage. Tschermaks miner. petrogr. Mitt., 7, 235-245.

———————, Paulitsch, P., & Walitzi, E. M. (1957) Die struchtur von Karinthin und einer barroisitschen hornblende. Tschermaks miner. petrogr. Mitt., 6, 215-225.

Hermes, O.D. (1970) Petrochemistry and coexistant mafic silicates from the Leckelenberg gabbro - metagabbro complex, North Carolina. Bull. Geol. Soc. Amer., 81, 137-161.

Heron, A. M. (1924) Soda bearing rocks of Nishengarh, Rajputana. Geol. Surv. India Records, 56, 179-197.

Hey, M. H. (1939) On the presentation of chemical analyses of minerals. Mineral. Mag., 25, 404-412.

———, (1954) A further note on the presentation of chemical analyses of minerals. Mineral. Mag., 30, 481-497.

Hezner, L. (1903) Ein Beitrag zur Kenntnis der Eklogite und Amphibolite. Min. Petr. Mitt., 22, 437-505.

Himmelberg, G. R., & Papike, J. J. (1969) Coexisting amphiboles from Blueschist facies metamorphic rocks. J. Petrology, 10, 102-114.

Hinrichsen, J. Th. (1968) Hydrothermal investigations and stability relations of synthetic gedrites. Mineral. Soc. I.M.A. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966),

Hodgson, A. A., Freeman, A. G., & Taylor, H. F. W. (1965) The thermal decomposition of amosite. Mineral. Mag., 35, 445-463.

Holgate, N. (1951) On crossite from Anglesey. Mineral. Mag., 29, 792-798.

Holloway, J. R. (1973) The system pargasite - H_2O - CO_2: a model for melting of a hydrous mineral with a mixed volatile fluid - I. Experimental results to 8 kbar. Geochim. Cosmochim. Acta, 37, 651-666.

———, & Burnham, C. W. (1972) Melting relations of basalt with equilibrium water pressure less than total pressure. J. Petrology, 13, 1-29.

Holm, R. F. (1971) Some garnets, pyroxenes and amphiboles from nepheline gneisses in Ghana. Am. Miner., 56, 2111-2122.

Howie, R. A. (1963) Kaersutite from the Lugar Sill, Ayrshire, and from alnöite breccia, Alnö Island, Sweden. Mineral. Mag.,

33, 716-719.

Hubaux, A (1969) Archival files of Geological data. Jour. Intern. Assoc. Math. Geol., 1, 41-52.

Huebner, J. S., & Papike, J. J. (1970) Synthesis and crystal chemistry of sodium - potassium richterite, $(Na,K)NaCaMg_5Si_8O_{22}(OH)_2$: a model for amphiboles. Am. Miner., 55, 1973-1992.

Iiyama, J. T. (1963) Synthèse hydrothermale à 750° C, 1000 bars dans la système Na_2O - MgO - Al_2O_3 - SiO_2 - H_2O d'amphibole orthorhombiques et monocliniques. C. R. Acad. Sci. Paris, 256, 966-967.

Iwasaki, M. (1963) Metamorphic rocks of the Motu - Bizan area eastern Shikoku. J. Fac. Sci. Tokyo Univ., 15, 1-90.

Jasmund, K., & Schafer, R. (1972) Experimentelle Bestim-mung der P - T Stabilitatsbereiches in der Mischkristallreiche Tremolite - Tschermakite. Contr. Mineral. and Petrology, 34, 101-115.

Kaiser, E. Die Diamantenwuste Sudwest Afrikas. 1, p.304.

Kamineni, D. C. (1973) X-ray and Mössbauer characteristics of a cummingtonite from Yellowknife, Distric of Mackenzie. Can. Mineral., 12, 230-232.

Kanisawa, S. (1964) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Kawano, Y. (1934) Chemical formula of basaltic hornblende. Proc. Imp. Acad. Japan, 10, 349-352.

Kempe, D. R. C. (1968) Kaersutite from minverite of Cornwall. Mineral. Mag., 36. 874-876.

Kesson, S., & Price, R. C. (1972) The major and trace element chemistry of kaersutite and its bearing on the petrogenesis of alkaline rocks. Contr. Mineral. and Petrology, 35, 119-124.

Kisch, H. J. (1969) Magnesiocummingtonite - $P2_1/m$: A Ca and Mn - poor clino-amphibole from New South Wales. Contr. Mineral. and Petrology, 21, 319-331.

_____, & Warnaars, F. W. (1969) Distribution of Mg and Fe in cummingtonite - hornblende and cummingtonite - actinolite pairs in metamorphic assemblages. Contr. Mineral. and Petrology, 24, 245-267.

Kitamura, M., & Morimoto, N. (1972) Crystal structure of kozulite and tetrahedral Al in amphiboles (abstr). Acta Crystallogr., A28, 71.

_____, & Tokonami, M. (1971) The crystal structure of kaersutite. Sci. Rep. Tohoku Univ., 11, 125-141.

Klein, C. Jr. (1964) Cummingtonite- grunerite series: a chemical, optical and X-ray study. Am. Miner., 49, 963-982.

_____, (1966) Mineralogy and petrology of the metamorphosed Wabush iron formation, Southeastern Labrador. J. Petrology, 7, 246-305.

_____, (1968) Coexisting amphiboles. J. Petrology, 9, 281-330.

_____, (1969) Two-amphibole assemblages in the system actinolite - hornblende - glaucophane. Am. Miner., 54, 212-237.

_____, & Ito, J. (1968) Zincian and manganoan amphiboles from Franklin, New Jersey. Am. Miner., 53, 1264-1275.

Knorring, O. von, & Kennedy, W. Q. (1958) The mineral paragenesis and metamorphic status of garnet-hornblende-pyroxene-scapolite gneiss from Ghana (Gold Coast). Mineral. Mag., 31, 846-859.

Krank, S. H. (1961) A study of phase equilibria in a metamorphic iron formation. J. Petrology, 2, 137-184.

Kreutz, S. (1908) Untersuchung der optischen Eigenschaften der Amphibolegruppe und ihre Abhangigkeit van der chemischen Zusammensetzung. Zeits. Krist., 49, 210.

Kohn, J. M., & Comeferro, J. F. (1955) Synthetic asbestos

investigations. II: X-ray and other data on synthetic fluor-richterite, edenite , and boron edenite. Am. Miner., 40, 410-421.

Moritnig, S. (1940) Ein Beitrag Zur Kenntnis uber den Marinthin Zentralblatt Min. Abt. A, 31-36.

_____ , (1965) Geochemistry of phosphorous - I. The replacement of Si^{4+} by P^{5+} in some rock-forming silicate minerals. Geochim. Cosmochim. Acta, 29, 361-371.

Kostyuk, E. A., & Sobolev, V. S. (1969) Pragenetic types of amphiboles of the hornblende-actinolite series in metamorphic rocks. Lithos, 2, 67-81.

Kovalenko, V. I. (.968) On the chemical composition, properties and mineral paragenesis of riebeckite and arfvedsonite. Mineral Spc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966), 261-284.

Kunitz, W. (1930) Isomorphieverhaltnisse in der Hornblene-gruppe. Neues. Jahrb. Min., 60, 171-230.

Kuno, H. (1938) On the occurrence of a primary cummingtonitic hornblende in some dacites from Japan. Proc. Imp. Acad. Tokyo. 14, 221-224.

Laitikari, A. (1920) Uber die petrographie und mineralogie der kalksteinlagerstatten von Parainen (Pargas). Bull. Comm. geol. Finl., 54, 113pp.

Lal, R. K. (1969) Paragenetic relations of aluminosilicates and gedrite from Fishtail Lake, Ontario, Canada. Lithos, 2, 187-196.

Larsen, E. S. (1938) The accuracy of chemical analyses of amphiboles and other silicates. Am. J. Sci., 35, 94-103.

_____, (1942) Alkalic rocks of Iron Hill, Gunnison County, Colorado. U. S. Geol. Surv. Prof. Paper, 197A.

_____, & Berman, H. (1934) The microscopic determination of nonopaque minerals. U. S. Geol. Surv. Bull. No. 848, 266pp.

Laudermilk, J. D., & Woodford, A. O. (1930) Soda-rich anthophyllite asbestos from Trinity County, California. Am. Miner., 15, 259-262.

Laughlin, A. W., Brookins, D. G., Rudo, A. N., & Causey, J. D. (1971) Late Cenozoic Basalts from the Bandera Lava Field, Valencia County, New Mexico. Geochim. Cosmochim. Acta, 35, 107-113.

Law, A. D. (1973) Critical evaluation of 'Statistical Best Fits' to Mössbauer spectra. Am. Miner., 58, 128-131.

Layton, W. (1965) Some aspects of optical properties and cell dimensions of amphiboles and pyroxenes. Neues Jb. Miner. Mh., 12, 369-379.

_____, & Phillips, R. (1960) The cummingtonite problem. Mineral. Mag., 32, 659-663.

Leake, B. E. (1962) On the non-existence of a vacant area in the Hallimond calciferous amphibole diagram. Jap. J. Geol. Geogr., 33, 1-13.

_____, (1965a) The relationship between tetrahedral aluminium and the maximum possible octahedral aluminium in natural calciferous and subcalciferous amphiboles. Am. Miner., 50, 843-851.

_____, (1965b) The relationship between the composition of calciferous amphibole and grade of metamorphism. In: 'Controls of Metamorphism', ed. Pitcher, W. S. and Flinn, G. W.

_____, (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

_____, (1971) On aluminous and edenitic hornblendes. Mineral. Mag., 38, 389-407.

Lee, D. E., Coleman, R. G., Bastron, H., & Smith, V. C. (1966) A two- amphibole glaucophane schist in the Franciscan

Formation, Canadero area, Sonoma County, California. Prof. Pap. U. S. Geol. Surv., 550-C, C148-157.

Le Maitre, R. W. (1969) Kaersutite bearing plutonic xenoliths from Tristan da Cunha, S. Atlantic. Mineral. Mag., 37, 185-197.

_____, (1973) Experiences with CLAIR: A computerised library of analysed igneous rocks. Chemical Geology, 12, 301-308.-

Linthout, K., & Kieft. C. (1970) Preliminary note on a mboziite of metamorphic origin. Mineral. Mag., 37, 629-631.

Litvin, A. L., Nichnik, T. L., & Ostapenko, S. S. (1973) X-ray and Mössbauer investigations of cation distribution in cataphorite (taramite). Geol. Vh., 33, 48-55.

_____, Yegoreva, L. N., & Kuts, V. P. (1972) Comparitive structural characteristics of hornblende from amphibolite and granulite metamorphic facies in the Ukranian Shield. Konst. Svoysta Miner., 6, 3-15.

_____, _____, & Tepikin, V. Ye. (1971) Structure and distribution of Mg - Fe^{2+} in hornblende from gneisses of the Rosa River area, Ukrainian Shield. Konst. Svoysta Miner., 5, 3-8.

Livingstone, A. (1967) A garnet peridotite and a garnet-amphibole pyroxenite from South Harris, Outer Hebrides, and their bearing on the South Harris eclogite facies status. Mineral. Mag., 36, 380-388.

Lorenzen, J. (1884) Untersuchungen grönlandischer Mineralien. Z. Krist., 11, 315-318.

Loudon, T. V. (1970) Some Geological data structures: Arrays networks, trees and forests. Systematics Association Spec. Vol. No. 3. 'Data Processing in Biology and Geology'. ed. Cutbill, J. L. 135-145.

Lovering, J. F., & White, A. J. R. (1969) Granulitic and eclogitic inclusions from basic pipes at Delegate, Australia.

Contr, Mineral. and Petrology, 21, 9-52.

Lukac, R. (1935) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Lupanova, P. P. (1943) Basaltic hornblende and augite from monchikite of Hibina Mountains. Trav. Inst. Petrogr. Akad. Sci. U.S.S.R., 6, 53.

Machatschki, F., & Walitzi, E. M. (1963) Hornblenden aus Eklogiten und Amphiboliten der Sudlichen Koralpe. Tschermaks miner. petrogr. Mitt., 8, 140-151.

Mason, B. (1953) Cummingtonite from Likonui River, Westland, New Zealand, Am. Miner., 38, 862-865.

_____, (1968a) Kaersutite from San Carlos, Arizona, with comments on the paragenesis of this mineral. Mineral. Mag., 36, 997-1002.

_____, (1968b) Eclogite xenoliths from volcanic breccia at Kakanui, New Zealand. Contr. Mineral. and Petrology, 19, 316-327.

Mathias, M. (1952) A note on two actinolites and a chlorite from the Pricska district, Cape Province. Trans. Geol. Soc. S. Africa., 55, 13-18.

Mauritz, B. (1911) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Meyer, H. O. A., & Brookins, D. G. (1971) Eclogite xenoliths from Stockdale Kimberlite, Kansas. Contr. Mineral. and Petrology, 34, 60-72.

Mikola, E., & Sahama, Th. G. (1936) The region to the south-west of the 'granulite series' in Lapland and its ultrabasics. Bull. comm. geol. Finl., 115, 357-371.

Mitchell, J. T., Bloss, D. F., & Gibbs, G. V. (1970) A refinement of the structure of actinolite. Am. Miner., 55, 302-303.

———, ———, ———, (1971) Examination of the actinolite structure and four other C2/m amphiboles in terms of double bonding. Z. Kristallogr., 133, 273-300.

Miyashiro, A. (1957) The chemistry, optics and genesis of the alkali amphiboles. J. Fac. Sci. Univ. Tokyo, 11, 57-83.

———, (1958) Regional metamorphism of the Gosaisyo-Takanuki district in the Central Abukuma Plateau. J. Fac. Sci. Univ. Tokyo, 11, 219-272.

Moore, P. B. (1969) Joesmithite: A novel amphibole crystal structure. Mineral. Soc. Amer. Spec. Paper, 2, 111-115.

Morgan, B. A. (1970) Petrology and mineralogy of eclogite and garnet amphibolite from Puerto Cabello, Venezuela. J. Petrology, 11, 101-145.

Morozewicz, J. (1923) O kilku amfibolach zelazzisto-alkalicznych. Spraw. Polsk. Inst. Geol., 2, 5-15.

———, (1926) Sur quelques amphiboles ferro-alcalines Compt. Rend. Conges Geol. Intern. Session XIII, 3, 1623.

Mössbauer, R. L. (1958) Kernresonanzfluorescent von Gammastrahlung in Ir^{191}. Z. Phys., 151, 124-143.

Mottana, A., Church, W. R., Edgar, A. D. (1968) Chemistry, mineralogy and petrography of an eclogite from the type locality (Saualpe, Austria). Contr. Mineral. and Petrology, 18, 338-346.

———, & Edgar, A. D. (1969) The significance of amphibole compositions in the genesis of eclogites. Lithos, 3, 37-49.

Mueller, R. F. (1960) Compositional characteristics and equilibrium relations in mineral assemblages of a metamorphosed iron formation. Am. J. Sci., 258, 449-497.

Naidu, P. R. J. (1954) Minerals of charnockites from India. Schweiz. Miner. petrogr. Mitt., 34, 204-279.

Nash, W. P., Carmichael, I. S. E., & Johnson, R. W. (1969) The mineralogy and petrology of Mount Suswa, Kenya. J. Petrology, 10, 409-439.

Nicholls, J., Carmichael, I. S. E.(1969) Peralkaline liquids: A petrological study. Contr. Mineral. and Petrology, 20, 268-294.

Nikitina, L. P., Pethevich, E. Z., & Sverdlova, O. V. (1973) Application of infrared studies of the OH-bonds to the determination of the octahedral site population in structures of amphiboles of the $(Ca,Na,K)_2(Fe^{2+},Fe^{3+},Mg,Al)_5((Si,Al)_4O_{11})_2(OH)_2$ composition. Geokhim. (Akad. Nauk. SSSR), 11, 1661-1668.

Nockolds, S. R. (1941) The Garabal Hill - Glen Fyne igneous complex. Q. Jl. geol. Soc. Lond., 96, 451-511.

Notley, M. C. (1972) The Peterlee IS/1 system. IBH United Kingdom Scientific Centre Rept., 0018. 20pp.

Novotny, M. (1949) On the chemical composition and physical properties of some Moravian amphiboles. Acta. Acad. Sci. Nat. Moravo-Silesiacae. Brno., 21, 24.

O'Hara, M. J. (1960) A garnet-hornblende-pyroxene rock from Glenelg, Inverness-shire. Geol, Mag., 97, 145-156.

_____, & Mercy, E. L. P. (1963) Petrology and petrogenesis of some garnetiferous peridotites. Trans. Roy. Soc. Edinburgh, 65, 251-314.

Ohashi, Y., & Burnham, W. (1972) Electrostatic and repulsive energies of the M1 and M2 cation sites in pyroxenes. J. Geophys. Res., 77, 5761-5766.

Olsen, E. (1967) Amphibole: first occurrence in a meteorite. Science, 156, 61-62.

_____, Huebner, J. S., Douglas, J. A. V., & Plant, A. G. (1973) Meteoritic amphiboles. Am. Miner., 58, 869-872.

Onuki, H. (1963) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with

their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

———, & Tiba, T. (1964) Ibid.

Osman, I. (1974) Matching of the storage organisation to usage pattern in relational data bases. Unpublished PhD thesis, Univ. Durham, England.

Oxburgh, E. R. (1964) Petrological evidence for the presence of amphibole in the upper mantle and its petrogenetic and geophysical implications. Geol. Mag., 101, 1-19.

Palache, C. (1894) On a rock from the vicinity of Berkely containing a new soda amphibole. Bull. Dept. Geol. Univ. Calif., 1, 161-192.

Palache, E. (1935) The minerals of Franklin and Sterling Hill, Sussex County, New Jersey. Prof. Paper U. S. Geol. Surv., 180, 135pp.

Papike, J. J., & Clark , J. R. (1967) Crystal chemical role of potassium and aluminium in a hornblende of proposed mantle origin (abstr). Geol. Soc. Amer. Prog. 1967, Ann. Meeting New Orleans (Geol. Soc. Amer. Spec. Paper, 115, 171).

———, ———, (1968) The crystal structure and cation distribution of glaucophane. Am. Miner., 53, 1156-1173.

———, & Ross, M. (1970) Gedrite: Crystal structures and intracrystalline cation distributions. Am. Miner., 55, 1945-1972.

———, ———, & Clark, J. R. (1969) Crystal-chemical characteristics of clinoamphiboles based on five new structure refinements. Mineral. Soc. Amer. Spec. Paper, 2, 117-136.

Parsons, A. L. (1930) A chemical and optical study of amphibole. Contr. Canadian Mineralogy, 29-33.

Perchuk, L. L., Pavlenko, A. S., & Vernadskiy, V. I. (1967) Effect of temperature on the distribution of some isomorphous components among coexisting minerals of alkalic rocks. Geochemistry International, 4, 850-869.

Perry, J. Jr. (1967) An application of linear algebra to petrologic problems. Part I, Mineral classification. Geochim. Cosmochim. Acta, 31, 1043-1073.

————, (1968) Representations of mineral chemical analyses in 11 dimensional space Part 2, Amphiboles. Lithos, 1, 307-321.

————, (1970) A general method for constructing the set of all end members of a mineral group. Am. Miner., 55, 305.

Phillips, R. (1963) The recalculation of amphibole analyses. Mineral. Mag., 33, 701-711.

————, (1966) Amphibole compositional space. Mineral. Mag., 35, 945-952.

————, & Layton, W. (1964) The calciferous and alkali amphiboles. Mineral. Mag., 33, 1097-1109.

————, & Rowbotham, G. (1968) Studies on synthetic alkali amphiboles. Mineral Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966) 249-253.

Prentice, F. J. (1967) Cation distribution in magnesioriebeckites and riebeckites by infrared spectroscopy. M.Sc. Thesis, Victoria Univ, Wellington, New Zealand.

Prewitt, C. J., Papike, J. J., & Ross, M. (1970) Cummingtonite: A reversible, nonquenchable transition from $P2_1/m$ to C2/m symmetry. Earth Planetary Sci. Letts., 8, 448-450.

Prider, R. T. (1939) Some minerals of the leucite rich rocks of the West Kimberly area, Australia. Mineral. Mag., 25, 373-387.

Prinz, M., & Nehru, C. E. (1970) Comments on 'Kaersutite from San Carlos, Arizona, with comments on the paragenesis of this mineral' by Brian Mason. Mineral. Mag., 37, 333-337.

Rabbit, J. C. (1948) A new study of the anthophyllite series. Am. Miner., 33, 263-323.

Ramachandra, Rao M. B. (1937) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Read, P. B. (1973) Metamorphic amphiboles from the chlorite zone of Central and Western Otago, New Zealand. Can. Mineral., 12, 147.

Ridley, I. (1971) The petrology of some volcanic rocks from the British Tertiary Province: The islands of Rhum, Eigg, Canna and Muck. Contr. Mineral. and Petrology, 32, 251-266.

Robinson, K., Gibbs, G. V., & Ribbe, P. H. (1970) A refinement of the crystal structure of pargasite. Am. Miner., 55, 307.

Robinson, P., & Jaffe, H. W. (1969) Chemographic exploration of amphibole assemblages from central Massachusetts and southwestern New Hampshire. Mineral. Soc. Amer. Spec. Paper, 2, 251-274.

———, ———, Ross, M., & Klein, C. Jr. (1971) Orientation of exsolution lamellae in clinopyroxenes and clinoamphiboles: considerations of optimal phase boundaries. Am. Miner., 56, 909-939.

———, Ross, M., & Jaffe, H. W. (1971) Composition of the anthophyllite - gedrite series, comparisons of gedrite and hornblende, and the anthophyllite - gedrite solvus. Am. Miner., 56, 1005-1041.

Rondolino, R. (1936) Sopra alcuni anfiboli manganesiferi di Praborna (San Marcel - Valle d'Aosta). Periodico Min. Roma, 7, 109-121.

Roonwall, C. S. (1972) Trace elements in the Singhbhum granite, India. Geologische Rund., 61, 282-301.

Roper, J., Osman, I., & Knight, J. L. (1973) A relational model of data. I.U.C.C. Computer Science Colloquin, Univ. of Kent.

Rose, H., & Fromme, J. (1932) Über ein neues Nephritvorkommen im Radautal im Hartz. Contr. Min. Abt. A., 301-313.

Ross, C. S. (1929) Is chromite always a magmatic segregation product? Econ. Geol., 24, 641-645.

Ross, M., Papike, J. J., & Shaw, K. W. (1969) Exsolution textures in amphiboles as indicators of subsolidus thermal histories. Mineral. Soc. Amer. Spec. Paper, 2, 275-299.

Sahlstein, Th. G. (1935) Petrographie der Eclogite-einschlusse in den Gneissen des südwestlichen Liverpool-Landes, in Ost-Grönland. Meddel. om Grönland, 95, 5-43.

Saito, H. (1963) Synthesis of asbestos by isomorphous replacement in fluor-richterite. J. Chem. Soc. Japan, 66, 18-21.

Savolahti, A. (1966) The differentiation of gabbro-anorthosite intrusions and the formation of anorthosites. Bull. comm. geol. Finl., 222, 173-197.

Saxena, S. K., & Ekström, T. K. (1970) Statistical chemistry of calcic amphiboles. Contr, Mineral, and Petrology, 26, 276-284.

Schalder, J. (1914) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol, Soc. Amer. Spec. Paper, 98, 210pp.

Schneider, C. (1891) Ibid.

Schreyer, W., & Seifert, F. (1968) Synthetic amphiboles in the system Na_2O - MgO - SiO_2 - H_2O and their significance for the chemistry of natural amphiboles. Mineral. Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting Cambridge

1966), 327-338.

Schubert, W. (1969) Chlorit-hornblende-felse des bergsträßer Odenwaldes und ihre phasenpetrologie. Contr. Mineral. and Petrology, 21, 295-310.

Schürmann, K. (1968) Synthesis and stability field of cummingtonite. Mineral. Soc. I.M.A. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966) 253-260.

Seifert, F., & Virgo, D. (1974) Temperature dependance of intracrystalline Fe^{2+}- Mg distribution in a natural anthophyllite. Carnie Inst. Year Book, 73, 405-411.

Seitsaari, J. (1952) An association of cummingtonite and hornblende. Ann. Acad. Sci. Fennicae, A, 30, 20pp.

Semet, M. P. (1973) A crstal chemical study of synthetic magnesihastingsite. Am. Miner., 58, 480-494.

Shido,F. (1958) Plutonic and metamorphic rocks of Yakaso and Iritono district in the Central Abukuma plateau. J. Fac. Sci. Univ. Tokyo, 11, 131-217.

_____, (1959) Notes on some rock-forming minerals (9) Hornblende bearing eclogite from Gongen-yama of Higashi-Akaisi in the Bessi District, Sikoku. J. Geol. Soc. Japan, 65, 701-703.

_____, Miyashiro, A. (1959) Hornblendes of basic metamorphic rocks. J. Fac. Sci. Univ. Tokyo, 12, 85-102.

Smith, J. V. (1959) Graphical representation of some amphibole compositions. Am. Miner., 44, 437-440.

Steuert, J., & Goldman, J. (1974) The relational data management system: A perspective. AGM-SICFIDET Workshop on data description, access and control. 26pp.

Stout, J. H. (1971) Four coexisting amphiboles from Telemark, Norway. Am. Miner., 56, 212-224.

_____, (1972) Phase petrology and mineral chemistry of coexisting amphiboles from Telemark, Norway. J. Petrology, 13, 99-145.

Streckeisen, A. (1954) Das nephelin syenit Massiv von Ditro (Siebenburgen). Schweiz. miner. petrogr. mitt., 34, 336-400.

Strens, R. G. J. (1966) Infrared study of cation ordering and clustering in some (Fe,Mg) amphibole solid solutions. Chem. Comm., 519-520.

Sueno, S., Cameron, M., Papike, J. J., & Prewitt, C. J. (1973) The high temperature crystal chemistry of tremolite. Am. Miner., 58, 649-664.

Sundius, N. (1946) The classification of hornblendes and the solid solution relations in the amphibole group. Arsbok. Sveriges Geologiska Undersoking, 40.

Sutherland, D. S. (1969) Sodic amphiboles and pyroxenes from fenites in East Africa. Contr. Mineral. and Petrology, 24, 114-135.

Taylor, H. P., & Coleman, R. G. (1968) O^{18}/O^{16} ratios of coexisting minerals in glaucophane bearing metamorphic rocks. Bull. Geol. Soc. Amer., 79, 1727-1756.

Tilley, C. E. (1957) Paragenesis of anthophyllite and hornblende from the Bancroft Area, Ontario. Am. Miner., 42, 412-416.

Tomita, K. (1962) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Topping, J. (1962) Errors of Observation and Their Treatment. 3rd (ed), Chapman and Hall, London, 119pp.

Troger, F., & Walitzai, E. K. (1965) Strukturuntersuchung an einer Hornblende aus dem chloritischen Gestein von Strallegg, Sudliche Koralpe. Tschl. Aktiebal. Atlas Diesel., 10, 233-240.

Turner, F. J. (1968) Metamorphic Petrology Mineralogical and Field Aspects. McGraw-Hill, New York, 403pp.

Uchimizu, M. (1966) Geology and petrology of alkali rocks from Dogo, Oki Islands. J. Fac. Sci. Tokyo Univ., 16, 85-159.

Valiquette, G., & Archambault, G. (1970) Les gabbros et les syénites du complexe de Brome. Can. Mineral., 10, 485-510.

Van der Plas, L., & Hugi, Th. (1961) A ferrian-sodium amphibole from Vals, Switzerland. Schweiz. miner. petrogr. Mitt., 41, 371-393.

Velde, B., Hervé, F., & Hornprobst, J. (1970) The eclogite - amphibolite transition at 650° c and 6.5 kbar pressure, as exemplified by basic rocks of the Uzerche area, central France. Am. Miner., 55, 953-974.

Velde, D. (1971) Les lamprophyres à feldspath alcalin et biotite minettes et roches voisines. Contr. Mineral. and Petrology, 30, 216-239.

Vincent, E. A. (1953) Hornblende - lamprophyre dykes of basaltic parentage from the Skaergaard area, east Greenland. Q. Jl. Geol. Soc. Lond., 109, 21-49.

Virgo, D. (1972) Preliminary fitting of ^{57}Fe Mossbauer spectra of synthetic Mg-Fe richterite. Carnegie Inst. Year Book, 71, 513-516.

Vlasov, K. A., Kuzmenko, M. V., & Eshova, E. N. (1966) The Lovozero Alkali Massif. Oliver and Boyd, Edinburgh, 627pp.

Volkov, V. P., Polykov, A. I., & Karakhanova, N. I. (1962) Chemical characteristics of rock forming minerals in the differentiated complex, Lovozero alkalic massif. Geochemistry Ann. Arbor., 561-570.

Warren, B. E. (1929) The structure of tremolite $H_2Ca_2Mg_5(SiO_3)_8$. Z. Kristallogr., 72, 42-57.

_____, & Modell, D. I. (1930) The structure of anthophyllite $H_2Mg_7(SiO_3)_8$. Z Kristallogr., 75, 161-178.

Washington, H. S., & Wright, F. E. (1908) On kaersutite from Linosa and Greenland. Am. J. Sci., 26, 187-211.

Weibull, M. (1896) On gedritskiffer from Sodra Dalarne. Geol. foren. Stockholm Forh., 18, 377-385.

White, A. J. R., Chappell, B. W., & Jakes, P. (1972) Coexisting clinopyroxene, garnet and amphibole from an 'eclogite', Kalammi, New Zealand. Contr. Mineral. and petrology, 34, 177-184.

Whitfield, H. J., & Freeman, A. G. (1967) Mössbauer study of amphiboles. J. Inorg. nucl. Chem., 29, 903-914.

Whittaker, E. J. W. (1949) The structure of Bolivian crocidolite. Acta Crystallogr., 2, 312-317.

_____, (1960) The crystal chemistry of the amphiboles. Acta Crystallogr., 13, 291-298.

_____, (1968) Classification of amphiboles. Mineral. Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966), 232-242.

_____, (1969) The structure of the orthorhombic amphibole holmquistite. Acta Crystallogr., B25, 394-397.

_____, (1971) Madelung energies and site preferences in amphiboles. Am. Miner., 56, 980-986.

_____, & Muntius, R. (1970) Ionic radii for use in geochemistry. Geochim. Cosmochim. Acta, 34, 945-956.

_____, & Zussman, J. (1961) The choice of axes in amphiboles. Acta Crystallogr., 14, 51-52.

Wiikstrom, A. (1970) Electron microprobe studies of the alteration of omphacite in eclogites from the Nordfjord area Norway. Norsk. geol. tidsskr., 50, 137-155.

Wilkins, R. W. T. (1970) Iron - magnesium distribution in the tremolite - actinolite series. Am. Miner., 55, 1993-1998.

_____, Davidson, L.R., & Ross, J. R. (1970) Occurrence and infrared spectra of holmquistite and hornblende from Mt. Marion, near Kalgoorlie, Western Australia. Contr. Mineral. and Petrology, 28, 280-287.

Wilkinson, J. F. G. (1961) Some aspects of the calciferous amphiboles, oxyhornblende, kaersutite and barkevite. Am. Miner., 46, 340-354.

Wilkinson, P. (1970) Automatic data handling in geochemistry and allied fields. Systematics Association Spec. Vol. No. 3, 'Data Processing in Biology and Geology', ed Cutbill, J. L.

Winchell, A. N. (1931) Further studies on the amphibole group. Am. Miner., 16, 250-266.

_____, (1945) Variations in composition and properties of the calciferous amphiboles. Am. Miner., 30, 27-50.

Winkler, H. G. F. (1967) Petrogenesis of Metamorphic Rocks. 2nd Ed. Springer- Verlag, Berlin, 237pp.

Wise, W. S. (1966) Zeolitic basanite from southwestern California. Bull. Volcan., 29, 235-252.

Witte, P., Langer, K., Seifert, F., & Schreyer, W. (1969) Synthetische Amphibole mit OH-Überschuß im System Na_2O - MgO - SiO_2 - H_2O. Naturwissenschaften, 56, 414-415.

Wolff, J. E. (1929) Mount Monadnock, Vermont - A syenite Hill. J. Geol., 37, 1-16.

Wolff, T. F. Von (1942) In: Leake, B. E. (1968) A catalog of analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 98, 210pp.

Wood, B. J., & Strens, R. G. J. (1969) Calculation of site preference energies and cation distributions in (Fe, Mg) amphiboles and pyroxenes from structural data. Am. Miner., 55, 316.

Woolley, A. R., Symes, R. F., & Elliott, C. J. (1972) Metasomatised (fenitized) quartzites from the Borralan Complex, Scotland. Mineral. Mag., 38, 819-836.

Yagi, K. (1953) On Kaersutite from Horotu, Sakhalin. Proc. Imp. Acad. Japan, 29, 239-245.

_____, Hariya, H., Onuma, K., & Fukushima, K. (1969) The phase relation of Kaersutite (abstr). Japan Mineral Soc., 1970 Ann. Meeting.

Yoshimura, T. (1940) in: Leake, B. E. (1968) A catalog of

analyzed calciferous and subcalciferous amphiboles together with their nomenclature and associated minerals. Geol. Soc. Amer. Spec. Paper, 28, 210pp.

Zambaonini, F. (1905) Ibid.

APPENDIX 1.

STRUCTURE AND SITE NOMENCLATURE OF THE AMPHIBOLES.

The basic structure of the amphiboles consists of two silicate chains, Fig. A1.1a, cross-linked to form a band of approximately hexagonally arranged SiO_4 tetrahedra, Fig. A1.1b. The band extends infinitely along the c axis. There are equal numbers of two distinct tetrahedrally co-ordinated sites designated T1 and T2. T1 is co-ordinated to three bridging oxygens plus one non-bridging oxygen and is smaller and more nearly regular than T2 which is co-ordinated to two bridging and two non-bridging oxygens. In detail the chains are kinked such that the angle O5 - O6 - O5 is less than 180^{o}, as in Fig. A1.1b. Collectively these tetrahedrally co-ordinated sites from part of the Z group of cations. An additional anion O3, the hydroxyl, occupies the centre of each hexagon. Viewed parallel to the c axis, the non-bridging oxygens plus O3 lie approximately in a plane, as do the Z group cations and the non-bridging oxygens, see Fig. A1.1c.

The silicate bands are arranged in layers parallel to (100). Along the b axis the bands alternate along a^{*}(the normal to (100)), to form layers. Layers are in turn stacked along a^{*} with non-bridging oxygens pointing alternatively towards and away from each other, Fig. A1.2.

Layers of silicate bands are held in place by cations. Five of these in three structurally distinct sites, two in M2, two in M1 and one in M3, are co-ordinated to the inward pointing non-bridging oxygens and O3. Each of the cations is in six fold co-ordination. This is accomplished by the displacement of the silicate bands above and below the cations by a stagger of approximately c/3. Six non-bridging oxygens form the co-ordination polyhedra around M2, but the M1 and M3 sites are co-ordinated to four non-bridging oxygens and two hydroxyls in *cis* and *trans* configuration respectively. The five cation sites are referred to collectively as the Y group.

Fig. A1.1. Site nomenclature of the silicate chain in the amphibole structure. Co-ordinates of the ions were taken from an X-ray refinement of grunerite (Finger 1969).

⊛ cations, o anions.

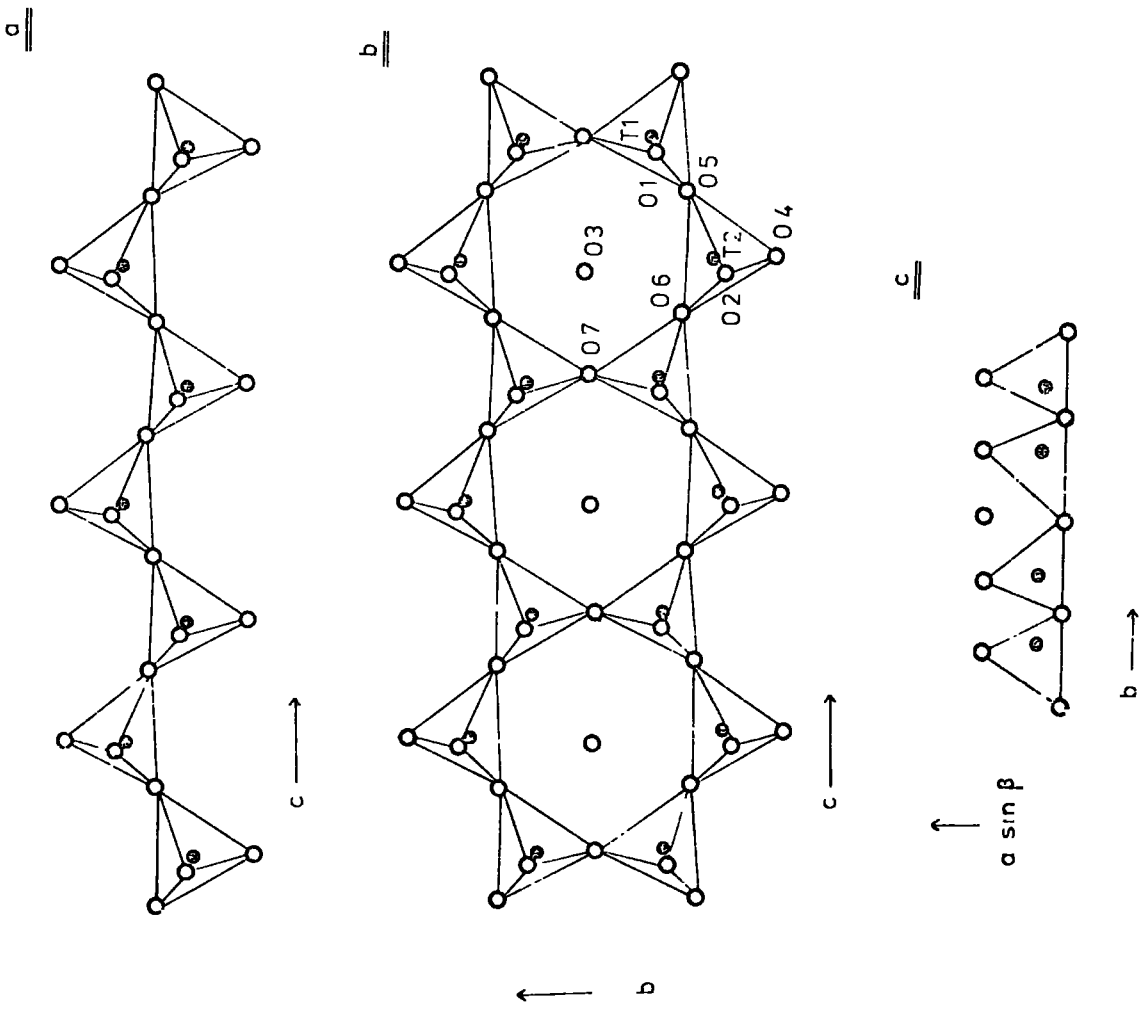
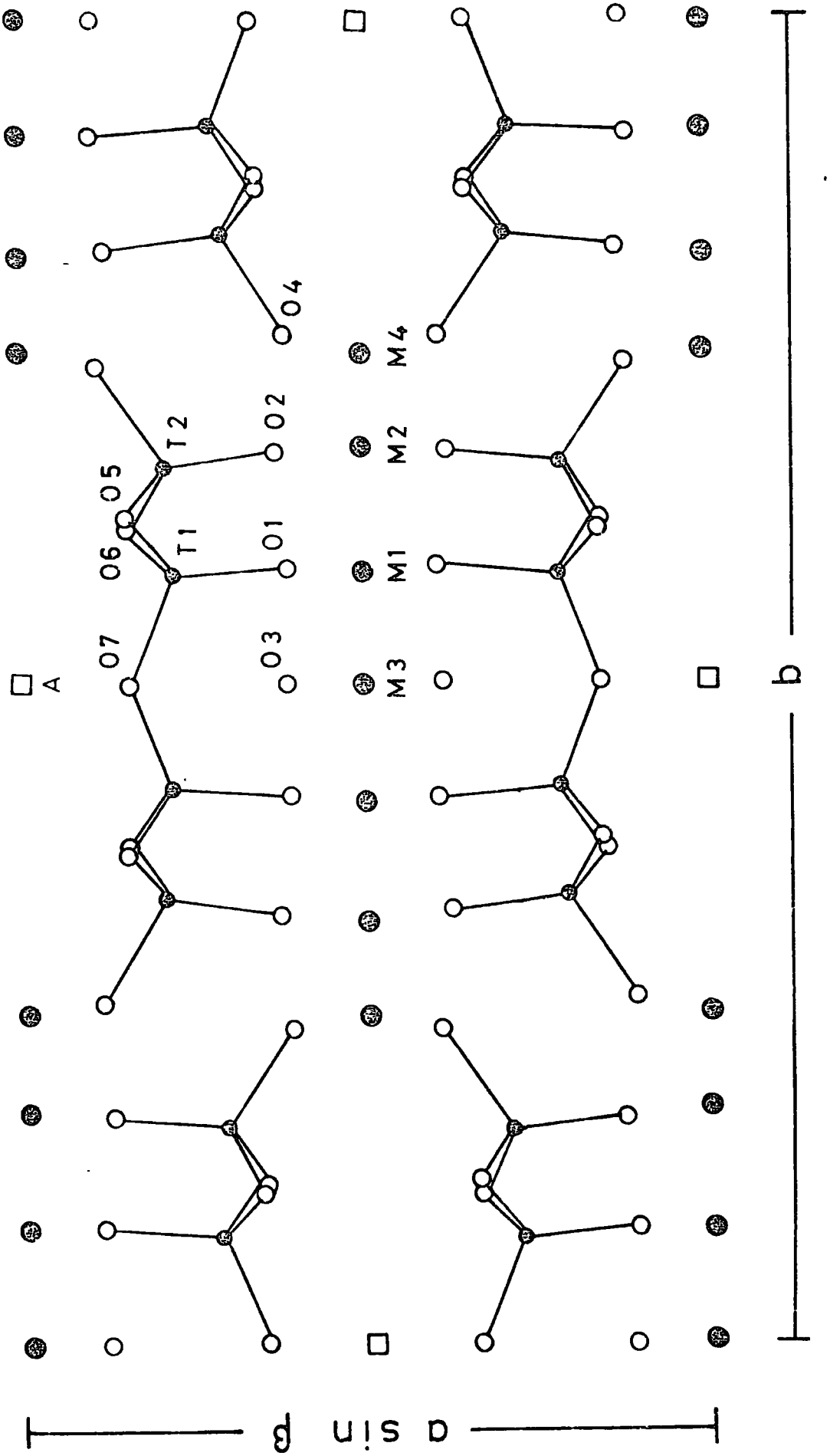

a
c
b
T1
O1
O5
O3
T2
O4
O6
O2
O7
b
c
c
a sin β
b

Fig. A1.2. Stacking of the silicate bands in the monoclinic amphibole grunerite. The co-ordinates of the ions were taken from Finger (1969).

● cation, o anion □ unoccupied A sites


a sin β
b
A
O7
O6
O5
T2
T1
O4
O2
O1
O3
M3
M1
M2
M4

One apex of both the upper and lower triangular faces of the Y group co-ordination polyhedra is orientated towards either +c or -c. Gibbs (1966) and Papike & Ross (1970) define a positively orientated cation strip as one in which the lower triangular face is orientated towards +c and conversly a negative strip has one apex of the lower face pointing towards -c.

Peripheral to the Y group cation strip the M^4 cation sites are co-ordinated to alternatively orientated silicate bands and serve to hold the layers together. Depending upon the ionic radius of the cation, the site may be in irregular 6,7 or 8 fold co-ordination. To accomplish this, displacement or distortion of the silicate bands is introduced. The two M^4 sites are normally referred to as the X group.

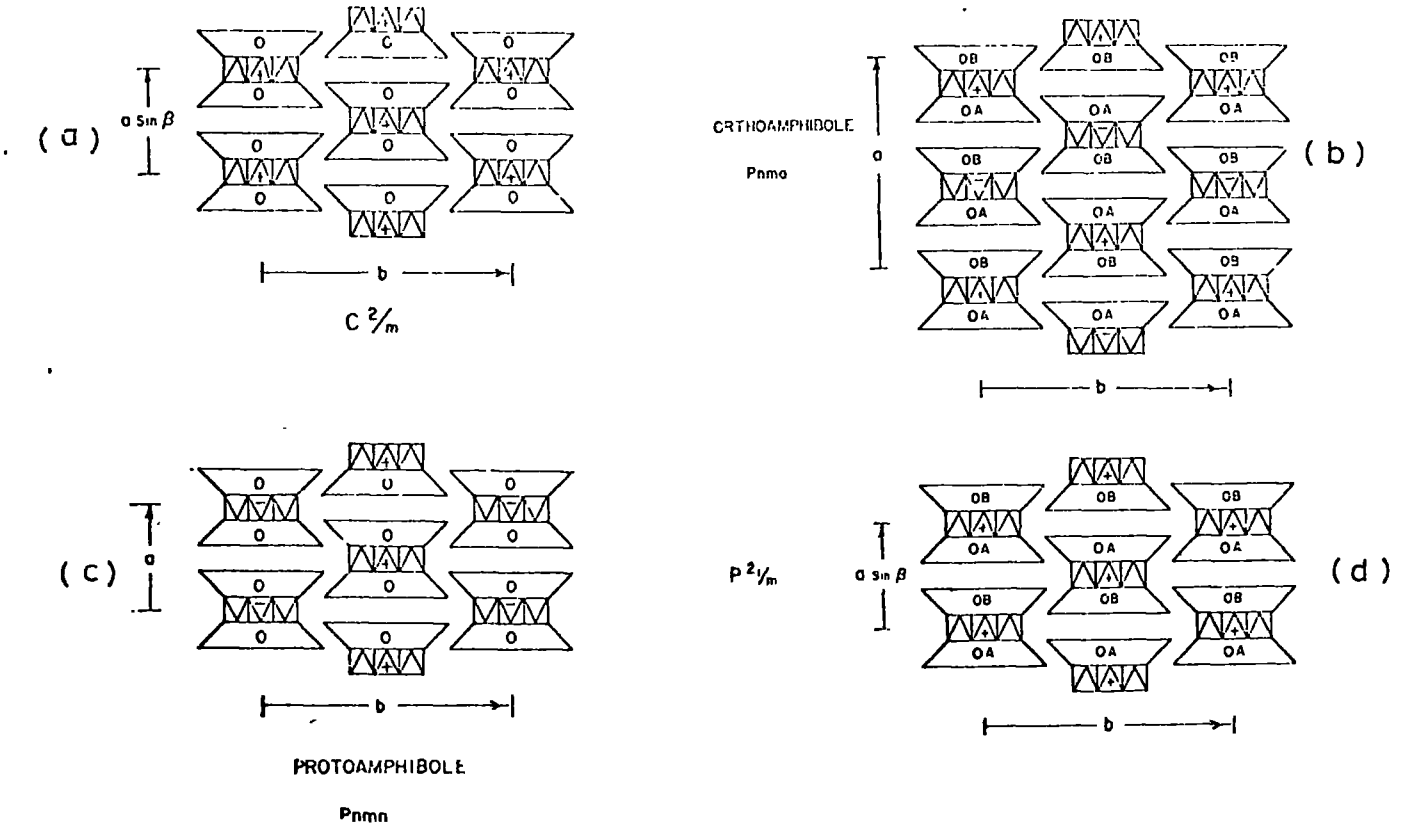
Lastly, the A sites situated at the back of the silicate bands may, or may not be occupied. When occupied the site is in 10 - 12 fold co-ordination in the clinoamphiboles or in 6 fold co-ordination in gedrite (Papike & Ross 1970).

Within the clinoamphibole half unit cell there are one A, two M^4, M2, M1, one M3, four T1, T2, two O3 and twenty oxygen sites. The general structural formula can be written as

$$A_{0-1}\ X_2\ Y_5\ Z_8\ O_{22}\ (OH)_2.$$

This brief description refers to the clinoamphiboles. A number of structural modifications leading to different space group symmetries have been recognised. By far the majority of clinoamphiboles belong to the space group C2/m or its geometrical equivalent I2/m (Whittaker & Zussman 1961). In these the cation strips are all similarily orientated and are co-ordinated to two identical silicate bands, Fig. A1.3a.

Fig. A1.3. Chain distortion and cation strip orientation in amphiboles belonging to the C2/M, Pnma, Pnmn and $P2_1/M$ space groups, after Papike & Ross (1970).



The clinoamphibole structure type, 'clino-anthophyllite' or primitive cummingtonite, was first recognised as an exsolved phase in tremolite by Bown (1965). Papike, Ross & Clark (1969) showed that the amphibole belonged to the space group $P2_1/m$. Apparently both Ca^{2+} and Mg^{2+} occupy the M^4 sites simultaneously. To bring about the observed co-ordination of the M^4 sites the silicate bands above and below the cation strip distort independantly forming two distinct bands designated A, B on Fig A1.3d. The co-ordination is such as to bring 7 oxygens (O2A,O2B,O4A,O4B,O6A,O6B,O5A) into close proximity to M^4. Primitive cummingtonite inverts to C2/m cummingtonite at temperatures above 40°C (Prewitt, Papike & Ross 1970).

Orthorhombic amphiboles, anthophyllite (Warren & Modell 1930; Finger 1970a,b), gedrite (Paike & Ross 1970) and holmquistite (Whittaker 1969; Finger & Ohashi 1974) have been assigned to the space group Pnma. Like the $P2_1/M$ cummingtonite the silicate bands above and below the cation strip distort independantly in order to co-ordinate the small Mg^{2+} or Li^+ cations in M^4. However, unlike $P2_1/M$ cummingtonite the orientation of the cation strip alternates, see Fig. A1.3b. An inversion from anthophyllite to either C_2/m or P_{2_1}/m cummingtonite, would involve a major rearrangement of the constituent ions.

Protoamphibole, a Mg^{2+}, Li^+ amphibole, synthesised by Gibbs, Bloss & Shell (1960) and investigated by Gibbs (1969) is also orthorhombic belonging to space group Pnmn. Unlike the other orthorhombic amphiboles there exists only one type of silicate band (Fig. A1.3c).

Lastly, Moore (1969) has described a unique Pb^{2+}, Be^{2+} rich clinoamphibole, joesmithite. Be^{2+} is completely ordered into one of the tetrahedrally co-ordinated cation sites of the silicate band causing the loss of the mirror symmetry plane. The amphibole belongs to space group P2/a.

APPENDIX 2. GENERAL ACCOUNT OF THE METHODS USED TO DETERMINE SITE POPULATIONS OF AMPHIBOLES.

A brief account of the methods by which published experimentally determined site populations have been obtained is given below, and the relative merits of the techniques are discussed.

A.2.1. X-ray diffraction.

The phenomenon of X-ray diffraction involves the scattering of X-rays by regions of high electron density (high scattering factors) corresponding to the location of atoms or ions in the crystal structure. Analysis of these regions of high electron density may in turn be related to the number of electrons in the ion occupying the structural site. In this way the location of ions with markedly different electron density may be inferred.

Unfortunately using electron density considerations alone it remains difficult and sometimes impossible to distinguish between ions with similar scattering factors or numbers of electrons, for example (Fe^{2+}, Mn^{2+}, Ti^{4+}), (Mg^{2+}, Al^{3+}, Si^{4+}, Na^{+}), and between ions of the same element in different oxidation states (Fe^{3+}, Fe^{2+}). Despite these difficulties a number of authors have made estimates of site populations of individual ions included in the above groups. This has been done by comparing the length of the bonds between the unknown cation species and the surrounding anion polyhedron with the bond lengths individual ions are known to make in other co-ordination polyhedra. By extrapolation between such extremes estimates of the distribution of Al^{3+}, Fe^{3+} in the Y group have been made (Whittaker 1949; Papike & Clark 1968; Mitchell *et al.* 1971), Fe^{2+}, Mn^{2+} in the Y group (Papike, Ross & Clark 1969), Fe^{2+}, Fe^{3+} in the Y group (Moore 1969) and Si^{4+}, Al^{3+} in the Z group (Papike, Ross & Clark 1969; Papike & Ross 1970; Kitamura & Tokonami 1971; Hawthorne & Grundy 1973a,b).

Such analyses have not been undertaken for every published X-ray site population.

A2.2. Infrared spectroscopy.

Burns (1965) demonstrated that in hydroxyl bearing minerals different cation species co-ordinated to the hydroxyl, altered the strength of the O - H bond. Qualitatively, the stronger the cation - oxygen bond the weaker the O - H bond. This variation in strength of the O - H bond causes slight alternations in the frequency of the hydroxyl fundamental band in the infrared.

Using a high resolution infrared spectrometer the hydroxyl fundamental band can be resolved into a number of absorption peaks corresponding to different cation - hydroxyl combinations. In the case of the amphiboles only cation species present in the two M1 and single M3 sites are co-ordinated to the hydroxyl. Provided the specific cation - OH combination can be paired with the absorption peak and the intensity of the peak related to the importance of the cation - OH combination, site populations for the 2M1 and M3 sites may be made. By subtraction from an atomic formula, populations for the M2 or M2 + M4 sites may be calculated.

In the simplest cases in which the 2M1, M3 sites are occupied by two cations (Fe^{2+}, Mg^{2+}) four absorption peaks have been recognised. This includes such compositions as tremolite - actinolite (Burns & Strens 1966; Burns & Greaves 1971), cummingtonite - grunerite (Burns & Strens 1966; Buckley & Wilkins 1971) and anthophyllite (Bancroft, Burns, Maddock & Strens 1966). More numerous peaks have been found in the alkali amphiboles in which Mg^{2+}, Fe^{2+}, Fe^{3+}, and Al^{vi} are possible occupants of the M1 and M3 sites (Bancroft & Burns 1969; Ernst & Wai 1970). Peak assignments have been given by the above authors. It should be noted however that errors in peak assignments have been made

(Burns & Greaves 1971, p. 2031).

An estimate of the site population of the M1, M3 sites may be made from the relative intensity of the absorption peaks. Early published results were based on peak height as a measure of the relative importance of cation combinations (Bancroft, Burns, Maddock & Strens 1966; Burns & Strens 1966; Burns & Prentice 1968; Bancroft & Burns 1969). Later workers (Burns & Law 1970; Wilkins 1970) demonstrated that the relative intensities of the peaks were more accurate if calculated from peak areas.

Unfortunately not all absorption peaks are non-overlapping. This leads to peak broadening and difficulties in estimating site populations. Strens in Bancroft & Burns (1969) found the calculated Fe^{2+}, Mg^{2+} population of the M1, M3 sites often exceeded the Fe^{2+} + Mg^{2+} content of the amphibole. This may be explained by the addition of overlapping absorption peaks, possibly from Mn^{2+} (Burns & Greaves 1971).

Lastly, Burns & Law (1970) have suggested that peak intensity may not be directly related to the proportion of the cation combinations present as had previously been assumed. Absorption peak intensity may be dependant upon the cation species present, thus the peak areas for $3Fe^{2+}$ and $3Mg^{2+}$ in the same sites need not be equal. The result of this effect on previously published site populations has not been evaluated.

A2.3. Mössbauer spectroscopy.

Mössbauer spectroscopy makes use of the absorption of gamma rays by a solid absorber, discovered by R.L. Mössbauer in 1957 (Mössbauer 1958). By moving the gamma ray source relative to the absorber the energy of the emitted gamma rays can be altered by the Doppler effect. If the absorption of gamma rays is measured during

the movement of the source relative to the absorber a Mössbauer spectrum is built up. For a detailed discussion of the method see Bancroft, Burns & Maddock (1967a,b).

While the Mössbauer effect has been observed for a large number of isotopes, from a geological point of view, only that shown by ^{57}Fe has been widely studied. Both ferrous and ferric iron species give rise to a Mössbauer spectrum of two absorption peaks, - a doublet. The position of the peaks, indicated by the chemical isomer shift (C.I. or δ), and the separation of the doublets from their midpoints, the quadruple splitting (Q.S. or Δ), can be related to measures of the electron density and to the asymmetry of the electric field about the nucleus respectively. Estimates of iron oxidation state, electronic configuration, co-ordination number, and the symmetry of the enclosing co-ordination polyhedron can be made. Provided the intensities of the absorption peaks can be related to the absolute number of iron cations occupying specific sites and the peaks themselves accurately assigned to cations, site populations may be calculated.

The Mössbauer spectra of cummingtonite - grunerite (Bancroft, Burns & Maddock 1967a,b; Hafner & Ghose 1971; Ghose & Weidner 1972) and anthophyllite (Bancroft, Burns & Maddock 1967b; Bancroft, Maddock, Burns & Strens 1966; Siefert & Virgo 1974) are essentially the same, consisting of two doublets assigned to ferrous iron in the structurally distinct (M4), (M2,M1,M3) sites. Site populations for Fe^{2+} among the X and Y groups can be calculated. An accuracy of $\pm$ 0.02 atoms has been claimed for the procedure (Hafner & Ghose 1971).

Mössbauer spectra of the remaining amphibole compositions have been interpreted in terms of the distribution of ferrous iron between the sites in the Y group, iron being absent in the X group. Two doublets assigned to (M2), (M1,M3) have been found in tremolite -

actinolite (Bancroft, Burns & Maddock 1967b). Later workers have been able to resolve the Mössbauer spectra into three doublets assigned to Fe^{2+} in the M2,M1, M3 sites (Burns & Greaves 1971; Greaves, Burns & Bancroft 1971).

Work on the alkali amphiboles in the series glaucophane - ferroglaucophane - ferroferriglaucophane - ferriglaucophane (Whitfield & Freeman 1967; Bancroft, Burns & Stone 1968; Bancroft & Burns 1969; Ernst & Wai 1970) has revealed three doublets. The doublets have been assigned to Fe^{2+} in M1, Fe^{2+} in (M2,M3) and Fe^{3+} in M2. Ernst & Wai (1970) have interpreted the single ferric doublet as evidence for the ordering of all ferric iron into the M2 sites and the lack of a third ferrous doublet as evidence for the absence of Fe^{2+} from M2. However, three ferrous doublets have been resolved for a magnesioriebeckite by Bancroft & Burns (1969).

In terms of the present study Mössbauer spectroscopy can yield site populations for Fe^{2+} in the X and Y groups and Fe^{3+} in the Y group. A large number of site populations derived from Mössbauer spectroscopy are included in Appendix 3.

A2.4. Comparison of X-ray diffraction, infrared and Mössbauer spectroscopy.

Included in the published site populations in Appendix 3 are a number of analyses in which site populations have been determined independantly by X-ray diffraction, infrared or Mössbauer spectroscopy. Unfortunately, the resultant site populations are not in all cases identical. Without a 'correct' standard from which site populations determined by differing techniques can be compared a somewhat arbitary choice has to be made between results.

In section A2.2 difficulties inherent in infrared spectroscopy were outlined. Burns & Greaves (1971) have discussed the

relative merits of infrared and Mössbauer spectroscopy in analysing site populations of the tremolite - actinolite series. The latter technique was found to be superior. In terms of the present study, Mössbauer spectroscopy can yield site populations relevant at group level and has been used in preference to infrared spectroscopy wherever appropriate.

A comparison of the site population of ferrous iron calculated from X-ray diffraction and Mössbauer spectroscopy has been made for tremolite (Burns & Greaves 1971) and cummingtonite Hafner & Ghose 1971). Both techniques yielded essentially similar site populations. Wherever appropriate X-ray site populations have been given preference in Appendix 3. Only in X-ray diffraction has it proved possible to recognise a large number of cations distributed between the A, X, Y and Z groups. For the remaining analyses Mössbauer or a combination of Mössbauer plus infrared site populations have been chosen in preference to those calculated from infrared spectroscopy alone.

APPENDIX 3.

PUBLISHED EXPERIMENTALLY DETERMINED AND CALCULATED CATION DISTRIBUTIONS.

The analyses are arranged by the authors name for the mineral viz anthophyllite (1 - 3), gedrite (4 - 5), holmquistite (6 - 7), cummingtonite - grunerite (8 - 42), tremolite - actinolite (43 - 55), pargasite - hastingsite (56 - 58), hornblende (59 - 60), richterite (61 - 64), kaersutite (65 - 66), tschermakite (67), Na-Ca amphibole (68), joesmithite (69), glaucophane - riebeckite (70 - 86).

Table A3.1. Published experimentally determined and calculated cation distributions.

	Ion	Group	Experimentally determined value	MINDAT A3 24(O)	MINDAT A3 23(O)	MINDAT A5 24(O)	MINDAT A5 23(O)
1	Fe^{2+}	X	1.41	1.76	1.84	1.76	1.84
	Fe^{2+}	Y	0.80	0.52	0.46	0.52	0.45
2	Fe^{2+}	X	1.39	0.00	0.00	1.68	1.67
	Fe^{2+}	Y	0.24	1.68	1.67	0.00	0.00
3	Mg^{2+}	X	0.70	1.92	1.88	0.64	0.60
	Mg^{2+}	Y	4.83	2.56	3.59	4.85	4.87
	Si^{4+}	Z	8.00	7.84	7.82	7.84	7.82
4	Na^{+}	A	0.52	0.31	0.51	0.32	0.51
	Fe^{2+}	X	1.30	1.74	1.92	1.74	1.93
	Mg^{2+}	X	0.62	0.00	0.00	0.00	0.00
	Ca^{2+}	X	0.04	0.04	0.04	0.04	0.04
	Na^{+}	X	0.02	0.22	0.03	0.22	0.03
	Fe^{2+}	Y	1.23	0.78	0.62	0.78	0.62
	Mg^{2+}	Y	2.41	2.97	3.00	2.97	3.00
	Al^{3+}	Y	1.36	1.22	1.36	1.24	1.36
	Si^{4+}	Z	5.96	5.87	5.95	5.87	5.95
	Al^{3+}	Z	2.04	2.13	2.05	2.03	2.05
5	Na^{+}	A	0.34	0.48	0.44	0.48	0.45
	Fe^{2+}	X	0.84	0.00	0.00	1.17	1.15
	Mg^{2+}	X	1.10	2.17	1.94	1.00	0.79
	Ca^{2+}	X	0.04	0.00	0.00	0.00	0.03
	Na^{+}	X	0.02	0.00	0.00	0.00	0.03
	Fe^{2+}	Y	0.42	2.23	2.21	0.06	0.06

	Mg^{2+}	Y	3.38	2.42	2.58	3.58	3.73
	Al^{3+}	Y	1.20	1.35	1.21	1.35	1.21
	Si^{4+}	Z	6.24	6.34	6.24	6.34	6.24
	Al^{3+}	Z	1.76	1.66	1.76	1.66	1.76
6	$Ca^{2+}+K^{+}$	A	0.04	0.00	0.00	0.00	0.00
	Mg^{2+}	X	0.10	0.64	0.62	0.00	0.00
	Li^{+}	X	1.80	0.00	0.00	1.79	1.79
	Na^{+}	X	0.06	0.03	0.03	0.03	0.03
	Mg^{2+}	Y	1.66	1.12	1.14	1.76	1.75
	Fe^{2+}	Y	1.50	0.23	0.24	1.39	1.41
	Al^{3+}	Y	1.84	1.84	1.83	1.84	1.82
7	Li^{+}	A	0.95	0.00	0.00	0.65	0.70
	Li^{+}	X	0.50	0.00	0.00	0.55	0.50
	Mg^{2+}	X	1.50	2.65	2.70	1.45	1.50
	Mg^{2+}	Y	5.00	3.80	3.79	5.00	5.00
8	Fe^{2+}	X	1.70	–	2.13	–	1.92
	Fe^{2+}	Y	1.95	–	1.82	–	2.02
9	Fe^{2+}	X	1.46	–	2.23	–	2.05
	Fe^{2+}	Y	1.00	–	0.43	–	0.61
10	Fe^{2+}	X	1.74	–	1.87	–	1.87
	Fe^{2+}	Y	3.40	–	3.39	–	3.39
11	Fe^{2+}	X	1.80	–	1.69	–	1.69
	Fe^{2+}	Y	3.75	–	3.81	–	3.81
12	Fe^{2+}	X	1.80	–	1.74	–	1.74
	Fe^{2+}	Y	4.87	–	4.85	–	4.85
13	Fe^{2+}	X	1.67	–	1.58	–	1.58
	Fe^{2+}	Y	4.28	–	4.22	–	4.22
14	Fe^{2+}	X	1.86	–	1.72	–	1.61

Fe^{2+}	Y	4.30	—	4.31	—	4.42
15 Mg^{2+}	X	0.03	0.00	0.00	0.00	0.00
Fe^{2+}	X	1.97	1.96	1.95	1.96	1.95
Mg^{2+}	Y	0.87	0.77	0.77	0.77	0.77
Fe^{2+}	Y	4.13	4.22	4.23	4.22	4.23
16 Fe^{2+}	X	1.90	2.16	2.10	2.16	2.10
Fe^{2+}	Y	3.40	3.41	3.42	3.41	3.42
17 Fe^{2+}	X	2.00	1.91	1.91	1.91	1.91
Fe^{2+}	Y	3.40	3.49	3.49	3.48	3.49
18 Fe^{2+}	X	1.72	—	1.82	—	1.68
Fe^{2+}	Y	3.25	—	3.10	—	3.24
19 Fe^{2+}	X	1.72	—	1.72	—	1.72
Fe^{2+}	Y	3.60	—	3.56	—	3.56
20 Fe^{2+}	X	1.74	—	1.63	—	1.51
Fe^{2+}	Y	2.15	—	2.13	—	2.24
21 Fe^{2+}	X	1.70	—	1.73	—	1.52
Fe^{2+}	Y	2.90	—	2.77	—	2.99
22 Fe^{2+}	X	1.78	—	1.55	—	1.55
Fe^{2+}	Y	3.85	—	3.94	—	3.94
23 Fe^{2+}	X	1.78	1.89	1.90	1.89	1.90
Fe^{2+}	Y	2.60	2.63	2.63	2.63	2.63
24 Fe^{2+}	X	1.73	1.80	1.91	1.67	1.78
Fe^{2+}	Y	2.68	2.50	2.44	2.63	2.57
25 Fe^{2+}	X	1.80	—	1.48	—	1.34
Fe^{2+}	Y	4.55	—	4.51	—	4.65
26 Fe^{2+}	X	1.68	1.99	1.93	1.99	1.93

Fe^{2+}	Y	2.20	2.17	2.20	2.17	2.20
27 Fe^{2+}	X	1.47	2.16	1.86	2.04	1.74
Fe^{2+}	Y	2.16	1.38	1.61	1.50	1.73
28 Fe^{2+}	X	1.58	—	1.75	—	1.75
Fe^{2+}	Y	1.50	—	1.36	—	1.36
29 Fe^{2+}	X	1.74	—	1.70	—	1.70
Fe^{2+}	Y	3.05	—	3.05	—	3.05
30 Fe^{2+}	X	1.58	1.86	1.86	1.53	1.53
Fe^{2+}	Y	1.95	1.69	1.69	2.02	2.02
31 Fe^{2+}	X	1.29	1.55	1.55	1.39	1.39
Mg^{2+}	X	0.10	0.00	0.00	0.00	0.00
Ca^{2+}	X	0.35	0.35	0.35	0.35	0.35
Mn^{2+}	X	0.16	0.00	0.00	0.16	0.16
Fe^{2+}	Y	0.81	0.56	0.56	0.71	0.71
Mg^{2+}	Y	3.95	4.05	4.05	4.05	4.05
Fe^{3+}	Y	0.14	0.19	0.19	0.19	0.19
Al^{3+}	Y	0.05	0.00	0.00	0.00	0.00
32 Fe^{2+}	X	1.74	—	1.52	—	1.34
Fe^{2+}	Y	1.75	—	1.74	—	1.92
33 Fe^{2+}	X	1.68	—	1.74	—	1.57
Fe^{2+}	Y	1.60	—	1.48	—	1.65
34 Fe^{2+}	X	1.74	—	1.68	—	1.51
Mg^{2+}	X	0.26	—	0.00	—	0.00
Fe^{2+}	Y	0.58	—	0.78	—	0.94
Mg^{2+}	Y	4.42	—	4.05	—	4.05
35 Fe^{2+}	X	1.70	1.79	1.79	1.79	1.79
Fe^{2+}	Y	1.60	1.57	1.57	1.57	1.57

36 Fe^{2+}	X	1.74	–	1.54	–	1.54
Fe^{2+}	Y	2.55	–	2.59	–	2.59
37 Fe^{2+}	X	1.70	–	1.61	–	1.50
Fe^{2+}	Y	3.35	–	3.26	–	3.36
38 Fe^{2+}	X	1.06	–	0.00	–	1.22
Fe^{2+}	Y	0.20	–	1.22	–	0.00
39 Fe^{2+}	X	1.65	–	1.88	–	1.88
Fe^{2+}	Y	0.82	–	0.67	–	0.67
40 Fe^{2+}	X	0.37	0.00	0.00	0.06	0.07
Fe^{2+}	Y	1.00	1.35	1.35	1.29	1.28
41 Ca^{2+}	X	0.18	0.18	0.18	0.18	0.18
Na^{+}	X	0.02	0.07	0.07	0.07	0.07
Mn^{2+}	X	1.56	1.67	1.74	1.67	1.74
Fe^{2+}	X	0.18	0.00	0.00	0.00	0.00
Mg^{2+}	X	0.06	0.00	0.00	0.00	0.00
Mg^{2+}	Y	4.14	4.10	4.13	4.10	4.13
Fe^{2+}	Y	0.37	0.54	0.55	0.54	0.55
Mn^{2+}	Y	0.49	0.35	0.29	0.35	0.29
42 Fe^{2+}	X	0.02	0.00	0.00	0.00	0.00
Mn^{2+}	X	0.98	0.00	0.00	0.96	0.96
Mg^{2+}	X	0.56	1.58	1.55	0.62	0.60
Ca^{2+}	X	0.38	0.36	0.36	0.36	0.36
Na^{+}	X	0.06	0.06	0.06	0.06	0.06
Mg^{2+}	Y	5.00	4.03	4.03	4.99	4.99
43 Fe^{2+}	Y	0.65	–	0.09	–	0.09
44 Ca^{2+}	X	1.76	1.74	1.73	1.74	1.73
Mn^{2+}	X	0.16	0.23	0.15	0.24	0.15

Na^{+}	X	0.08	0.02	0.10	0.02	0.10
Mg^{2+}	Y	1.88	1.95	1.94	1.95	1.94
Fe^{2+}	Y	2.72	2.53	2.52	2;53	2.52
Fe^{3+}	Y	0.32	0.31	0.38	0.31	0.38
Al^{3+}	Y	0.04	0.13	0.00	0.13	0.00
Si^{4+}	Z	7.68	7.76	7.71	7.76	7.71
Al^{3+}	Z	0.32	0.24	0.29	0.24	0.29
45 Fe^{2+}	Y	1.80	—	1.59	—	1.59
46 Fe^{2+}	X	0.00	0.23	0.27	0.23	0.27
Fe^{2+}	Y	2.86	2.64	2.62	2.64	2.62
47 Fe^{2+}	X	0.00	0.07	0.05	0.08	0.06
Fe^{2+}	Y	0.73	0.69	0.71	0.69	0.71
48 Fe^{2+}	Y	2.15	—	1.94	—	1.94
49 Fe^{2+}	Y	2.01	—	1.91	—	1.91
50 Fe^{2+}	Y	1.45	—	1.27	—	1.26
51 Fe^{2+}	X	0.00	—	0.14	—	0.14
Fe^{2+}	Y	2.40	—	2.29	—	2.29
52 Fe^{2+}	X	0.00	—	0.06	—	0.06
Fe^{2+}	Y	0.48	—	0.45	—	0.45
53 Fe^{2+}	Y	0.85	—	0.40	—	0.40
54 Fe^{2+}	Y	0.75	0.38	0.36	0.65	0.63
55 Ca^{2+}	X	1.90	1.78	1.88	1.78	1.88
Na^{+}	X	0.10	0.00	0.05	0.00	0.05
Mg^{2+}	Y	5.00	4.91	4.97	4.91	4.97
56 Mg^{2+}	Y	3.50	3.48	3.48	3.48	3.48
Fe^{2+}	Y	0.56	0.60	0.60	0.55	0.60

Ti^{4+}	Y	0.08	0.06	0.06	0.06	0.06
Al^{3+}	Y	0.16	0.14	0.16	0.18	0.16
Fe^{3+}	Y	0.72	0.72	0.72	0.72	0.72
57 Ca^{2+}	X	2.00	2.00	2.00	2.00	1.95
Mg^{2+}	Y	3.33	3.28	3.28	3.29	3.28
Fe^{2+}	Y	1.10	1.09	1.09	1.09	1.04
Al^{3+}	Y	0.60	0.59	0.59	0.59	0.59
58 Fe^{2+}	Y	1.36	1.06	1.09	1.06	1.09
59 Na^{+}	A	0.60	0.47	0.46	0.47	0.46
K^{+}	A	0.40	0.38	0.38	0.38	0.38
Ca^{2+}	X	1.63	1.61	1.61	1.61	1.61
Na^{+}	X	0.26	0.39	0.39	0.39	0.39
Fe^{2+}	Y	1.35	1.41	1.36	1.37	1.36
Mg^{2+}	Y	2.78	2.81	2.81	2.81	2.81
Ti^{4+}	Y	0.48	0.49	0.48	0.48	0.48
Al^{3+}	Y	0.38	0.28	0.28	0.28	0.27
Al^{3+}	Z	2.04	2.11	2.11	2.11	2.11
60 Mg^{2+}	Y	2.64	2.51	2.50	2.51	2.50
Fe^{2+}	Y	0.87	1.01	1.01	1.01	1.01
Fe^{3+}	Y	0.42	0.47	0.47	0.47	0.47
Ti^{4+}	Y	0.15	0.15	0.15	0.15	0.15
Al^{3+}	Y	0.91	0.86	0.83	0.86	0.84
61 Fe^{2+}	Y	4.51	4.47	4.47	4.47	4.47
Fe^{3+}	Y	0.49	0.48	0.48	0.48	0.48
62 K^{+}	A	1.00	1.02	1.07	1.03	1.05
Ca^{2+}	X	1.00	1.09	1.06	1.09	1.06
Na^{+}	X	1.00	0.60	0.73	0.60	0.73
Fe^{2+}	Y	0.29	0.29	0.08	0.29	0.08
Mg^{2+}	Y	4.53	4.27	4.49	4.55	4.49

Ti^{4+}	Y	0.17	0.38	0.37	0.38	0.37
Mn^{2+}	Y	0.01	—	—	—	—
63						
Na^{+}	A	1.00	1.08	1.09	1.08	1.09
Ca^{2+}	X	0.90	0.90	0.90	0.90	0.90
Na^{+}	X	1.02	0.97	0.97	0.97	0.96
Fe^{2+}	X	0.08	0.13	0.13	0.13	0.13
Mg^{2+}	Y	3.41	3.45	3.45	3.45	3.45
Fe^{2+}	Y	1.59	1.55	1.55	1.55	1.55
64						
Na^{+}	A	1.00	1.00	1.00	1.00	1.00
Ca^{2+}	X	1.00	1.00	1.00	1.00	1.00
Na^{+}	X	1.00	1.00	1.00	1.00	1.00
Mg^{2+}	Y	5.00	5.00	5,00	5.00	5.00
65						
Na^{+}	A	0.73	0.67	0.37	0.61	0.37
K^{+}	A	0.25	0.25	0.25	0.25	0.25
Ca^{2+}	X	1.72	1.72	1.67	1.72	1.67
Mg^{2+}	X	0.11	0.00	0.00	0.00	0.00
Fe^{3+}	X	0.05	0.00	0.00	0.00	0.00
Ti^{4+}	X	0.02	0.00	0.00	0.00	0.00
Fe^{2+}	X	0.02	0.22	0.00	0.22	0.00
Al^{3+}	X	0.02	0.00	0.00	0.00	0.00
Mg^{2+}	Y	2.32	2.40	2.33	2.40	2.33
Al^{3+}	Y	0.47	0.49	0.22	0.48	0.22
Fe^{3+}	Y	0.99	1.05	1.01	1.05	1.01
Fe^{2+}	Y	0.59	0.41	0.61	0.41	0.61
Ti^{4+}	Y	0.63	0.66	0.65	0.66	0.65
Si^{4+}	Z	5.76	5.74	5.56	5.74	5.56
Al^{3+}	Z	2.24	2.26	2.44	2.26	2.44
66						
Na^{+}	A	0.54	0.54	0.38	0.54	0.38
K^{+}	A	0.43	0.43	0.42	0.43	0.42
Ca^{2+}	X	1.92	1.86	1.86	1.86	1.86

Fe^{3+}	X	0.02	0.00	0.00	0.00	0.00
Mg^{2+}	X	0.02	0.14	0.00	0.14	0.00
Fe^{3+}	Y	1.03	1.06	1.03	1.06	1.03
Mg^{2+}	Y	3.08	3.05	3.09	3.05	3.09
Al^{3+}	Y	0.37	0.37	0.11	0.37	0.11
Ti^{4+}	Y	0.51	0.52	0.50	0.52	0.50
Si^{4+}	Z	5.88	5.88	5.70	5.88	5.70
Al^{3+}	Z	2.12	2.12	2.30	2.12	2.30
67 Ca^{2+}	X	1.86	1.86	1.87	1.86	1.87
Na^{+}	X	0.10	0.00	0.13	0.00	0.13
Mg^{2+}	X	0.02	0.00	0.00	0.00	0.00
Mn^{2+}	X	0.02	0.00	0.00	0.00	0.00
Fe^{2+}	Y	2.10	2.01	2.13	2.01	2.13
Mg^{2+}	Y	1.20	1.23	1.22	1.23	1.22
Al^{3+}	Y	1.30	1.32	1.29	1.37	1.30
Fe^{3+}	Y	0.30	0.30	0.30	0.30	0.30
Ti^{4+}	Y	0.10	0.10	0.10	0.10	0.10
Si^{4+}	Z	6.00	6.05	6.00	6.05	6.00
Al^{3+}	Z	2.00	1.95	2.00	1.95	2.00
68 Co^{2+}	X	0.74	0.00	0.00	0.20	0.21
Co^{2+}	Y	4.82	5.20	5.20	5.00	5.00
Na^{+}	X	1.26	2.00	2.00	1.80	1.79
69 Ca^{2+}	A	0.60	1.30	1.34	0.61	0.81
Pb^{2+}	A	0.00	0.00	0.00	0.40	0.40
Ca^{2+}	X	2.00	1.60	1.57	2.00	2.00
Mg^{2+}	Y	2.46	2.73	2.75	2.46	2.46
Fe^{3+}	Y	2.13	1.87	1.87	1.69	1.69
Fe^{2+}	Y	0.71	0.39	0.37	0.71	0.71
Si^{4+}	Z	6.00	6.70	6.73	6.00	6.00
Be^{2+}	Z	2.00	0.00	0.00	2.01	2.01

70

Fe^{2+}	Y	1.76	1.69	1.65	1.69	1.65
Fe^{3+}	Y	1.82	1.96	1.92	1.97	1.92
71						
Fe^{2+}	X	0.00	0.00	0.00	0.00	0.00
Mg^{2+}	X	0.00	0.00	0.00	0.00	0.00
$FeFe^{2+}$	Y	2.76	2.78	2.80	2.78	2.80
Fe^{3+}	Y	1.93	1.92	1.93	1.92	1.93
Mg^{2+}	Y	0.30	0.30	0.30	0.30	0.30
72						
Fe^{2+}	Y	2.58	2.46	2.49	2.46	2.49
Fe^{3+}	Y	2.00	2.09	2.18	2.13	2.17
73						
Fe^{2+}	Y	2.28	2.52	2.51	2.52	2.51
Fe^{3+}	Y	1.87	1.63	1.63	1.63	1.63
74						
Fe^{2+}	Y	2.59	2.93	2.90	2.93	2.90
Fe^{3+}	Y	2.10	2.02	1.99	1.92	1.94
75						
Fe^{2+}	Y	0.00	0.00	0.05	0.00	0.06
Fe^{3+}	Y	2.29	2.34	2.30	2.34	2.29
76						
Mg^{2+}	Y	0.89	1.02	1.04	1.02	1.04
Fe^{2+}	Y	2.01	1.85	1.88	1.85	1.88
Fe^{3+}	Y	2.10	2.06	2.10	2.06	2.09
77						
Fe^{2+}	Y	1.11	0.75	0.71	0.75	0.71
Fe^{3+}	Y	1.31	1.56	1.58	1.56	1.58
78						
Fe^{2+}	Y	1.22	1.24	1.17	1.24	1.17
Fe^{3+}	Y	0.80	0.85	0.85	0.85	0.85
79						
Fe^{2+}	Y	1.36	1.43	1.44	1.44	1.44
Fe^{3+}	Y	0.51	0.46	0.46	0.46	0.46
80						
Fe^{2+}	Y	1.19	1.23	1.23	1.23	1.23
Fe^{3+}	Y	1.15	1.15	1.15	1.15	1.15

81

Fe^{2+}	Y	1.33	1.44	1.44	1.44	1.44
Fe^{3+}	Y	0.26	0.17	0.17	0.17	0.17
82						
Fe^{2+}	X	0.00	0.00	0.00	0.00	0.00
Fe^{2+}	Y	1.57	1.60	1.60	1.60	1.60
83						
Fe^{2+}	Y	0.76	0.43	0.63	0.42	0.63
Fe^{3+}	Y	1.66	1.88	1.79	1.88	1.79
84						
Na^{+}	X	1.38	1.38	1.39	1.38	1.39
K^{+}	X	0.13	0.00	0.00	0.00	0.00
Ca^{2+}	X	0.17	0.17	0.17	0.17	0.17
Mg^{2+}	X	0.25	0.00	0.00	0.00	0.00
Mg^{2+}	Y	2.82	3.05	3.05	3.05	3.05
Fe^{2+}	Y	2.14	1.95	1.94	1.94	1.94
Al^{3+}	Y	0.02	0.00	0.00	0.00	0.00
85						
Fe^{2+}	X	0.00	0.08	0.00	0.09	0.00
Fe^{2+}	Y	1.11	1.05	1.12	1.04	1.12
86						
Na^{+}	X	1.96	1.80	1.80	1.80	1.80
Ca^{2+}	X	0.04	0.20	0.20	0.20	0.20
Mg^{2+}	Y	2.39	2.38	2.37	2.38	2.37
Fe^{2+}	Y	0.61	0.70	0.69	0.70	0.69
Fe^{3+}	Y	0.18	0.20	0.30	0.20	0.30
Al^{3+}	Y	1.82	1.66	1.53	1.66	1.53
Si^{4+}	Z	8.00	7.91	7.88	7.91	7.88

Table A3.2. Source of the experimentally determined cation distributions, relevant chemical analyses and additional information.

No.	Source of site populations	Source of analysis	Additional data
1	Bancroft et al. (1966), Table 2, 31.69% Fe(II).	Tilley (1957)	Burns & Law (1970)
2	Bancroft et al. (1966), Table 2, 23% Fe (II).	Rabbit (1948)	Bancroft, Burns & Haddock (1967b), Burns & Law (1970).
3	Finger (1970b), Table 26.	Rabbit (1948)	Finger (1970a) Seifert & Virgo (1974)
4	Papike & Ross (1970), Tables 7, 11, no. 002.	Robinson & Jaffe (1969)	
5	Papike & Ross (1970), Tables 7, 11, no, 001.	Papike & Ross (1970)	
6	Whittaker (1969), Table 1.	Knorring & Hornung (1961)	Law (1973)
7	Gibbs (1969)	Gibbs (1969)	
8	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 10-85	
9	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 7-482	Ghose & Weidner (1972)
10	Hafner & Ghose (1971), Table 6	Mueller (1960) no. B19	
11	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. B16	
12	Bancroft, Burns & Haddock (1967a), Table 4, no. 95.3% Fe(II).	Mueller (1960) no. 1B	Burns & Strens (1966), Bancroft, Burns & Haddock (1967b) Hafner & Ghose (1971)

13	Bancroft, Burns & Maddock (1967a), Table 4, no. 65.0% Fe(II).	Mueller (1960) no. 2B	Bancroft, Burns & Maddock (1967 b), Hafner & Ghose (1971)
14	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. E17	
15	Finger (1969)	Klein (1964) no. 1	Bancroft, Burns & Maddock (1967 a,b), Finger & Zoltai (1967), Hafner & Ghose (1971)
16	Hafner & Ghose (1971), Table 6.	Klein (1964) no. 9A.	
17	Whitfield & Freeman (1967), Table 2.	Hodgson et al. (1965), no. PHS 5.	
18	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 10-169	
19	Hafner & Ghose (1971) Table 6.	Mueller (1960) no. E13	
20	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 10-158	
21	Ghose & Hellner (1959)	Mueller (1960) no. DH 10-131	Hafner & Ghose (1971)
22	Hafner & Ghose (1971), Table 6	Mueller (1960) no. E14	
23	Hafner & Ghose (1971), Table 6.	Klein (1964) no. 11A	
24	Bancroft, Burns & Maddock (1967a), Tables 3,4, no. 63.0% Fe(II).	Klein (1964) no. 7	Bancroft, Burns & Maddock (1967b)
25	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. 9B	

26	Hafner & Ghose (1971), Table 6.	Klein (1964) no. 10A	
27	Bancroft, Burns & Haddock (1967a), Tables 3,4 no. 51.0% Fe(II).	Mason (1953)	Bancroft, Burns & Haddock (1967b).
28	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 10-95	
29	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. 6B	
30	Hafner & Ghose (1971) Table 6.	Butler (1969) no. 205	
31	Buckley & Wilkins (1971), Table 3.	Buckley & Wilkins (1971), Table 1	
32	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH7-490	
33	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. DH 7-484	
34	Fischer (1966), Table 1.	Ghose (1961)	Ghose (1961)
35	Hafner & Ghose (1971) Table 6.	Butler (1969) no. 264	
36	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. B-22A	
37	Hafner & Ghose (1971), Table 6.	Mueller (1960) no. CL-1	
38	Hafner & Ghose (1971), Table 6.	Kisch (1969) no. 1	Ghose & Weidner (1972)
39	Bancroft, Burns & Haddock (1967a) Tables 3,4, no. 118125.	Ghose & Weidner (1972)	Bancroft et al. (1966), Bancroft, Burns & Haddock (1967b), Ghose & Weidner (1972)

40	Bancroft, Burns & Maddock (1967a) Tables 3,4, no. 19.7% Fe(II).	Klein (1964), no. 4	Bancroft, Burns & Maddock (1967b)
41	Papike, Ross & Clark (1969)	Klein (1964), no. 2	
42	Papike, Ross & Clark (1969)	Ross, Papike & Shaw (1969), no. 115046	
43	Wilkins (1970)	Mueller (1960), no. DH 1-21	
44	Mitchell et al. (1971), Table 4.	Mitchell et al. (1971)	Mitchell et al. (1970), Burns & Greaves (1971
45	Wilkins (1970).	Mueller (1960), no. DH 7-445.	
46	Burns & Greaves (1971), Table 5.	Klein (1966) no. 11B.	Wilkins (1970)
47	Burns & Greaves (1971), Table 5.	Burns & Greaves (1971), no. 80714	Wilkins (1970)
48	Wilkins (1970).	Mueller (1960), no. DH 10-158	
49	Wilkins (1970).	Mueller (1960) no. B20	
50	Wilkins (1970).	Mueller (1960) no. 96	
51	Burns & Greaves (1971), Table 5.	Mueller (1960), no. 12BA	Burns & Strens (1966), Wilkins (1970)
52	Burns & Greaves (1971), Table 5.	Burns & Greaves (1971), no. 14785	Burns & Strens (1966)
53	Wilkins (1970).	Mueller (1960), no. F1.	
54	Burns & Greaves (1971), Table 5,	Klein (1966), no. 6.	Wilkins (1970)
55	Papike, Ross & Clark (1969).	Papike, Ross & Shaw (1969), no. 621.	

56	Semet (1973), no. U-1236.	calculated	
57	Robinson et al. (1970).	calculated	
58	Burns & Greaves (1971), Table 5.	Burns & Greaves (1971) no.4.	
59	Papike, Ross & Clark (1969).	calculated	Papike & Clark (1967)
60	Trozer & Walitzi (1965)	calculated	
61	Virgo (1972), Table 52.	calculated	
62	Papike, Ross & Clark (1969).	Prider (1939)	
63	Cameron & Gibbs (1971).	calculated	
64	Cameron & Gibbs (1971).	calcuated	
65	Kitamura & Tokanami (1971), Table 3.	Kitamura & Tokanami (1971)	
66	Hawthorne & Grundy (1973b).	Hawthorne & Grundy (1973b).	
67	Hawthorne & Grundy (1973a).	Hawthorne & Grundy (1973a).	
68	Gibbs (1966).	Gier, Cox & Young (1964), no. 3.	
69	Moore (1969).	calculated	
70	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. SW-6.	
71	Bancroft, Burns & Stone (1968).	Bancroft & Burns (1969), no. 5.	Burns & Prentice (1968), Bancroft & Burns (1969).
72	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. P-1.	
73	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. LC-3.	
74	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. LC-1.	

75	Bancroft & Burns (1969)	Bancroft & Burns (1969), no. 4.	
76	Burns & Prentice (1968)	Hodgson et al. (1965), no. L483.	
77	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. 5 C.	
78	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. 409.	
79	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. 423.	
80	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. 8.	
81	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. SL C-5	
82	Bancroft & Burns (1969).	Bancroft & Burns (1969), no. 3.	
83	Ernst & Wai (1970), Tables 2,5.	Ernst & Wai (1970), no. C-4980.	
84	Whittaker (1949)	Whittaker (1949)	Burns & Prentice (1968), Bancroft & Burns (1969)
85	Bancroft & Burns (1969);	Bancroft & Burns (1969), no. 2.	
86	Papike & Clark (1968).	Papike & Clark (1968)	Bancroft & Burns (1969), Ernst & Wai (1970)

APPENDIX 4.

DESCRIPTION AND LISTING OF THE ALLOCATION PROGRAM MINDATA5.

Program Function.

Starting from a chemical analysis MINDATA5 may be used to calculate an atomic formula for an amphibole, assuming an anion base of 24 or 23 oxygens. The ions are allocated to groups of sites using an allocation scheme derived from published site populations determined by X-ray diffraction infrared or Mössbauer spectroscopy (Chapter 2). In addition, MINDATA5 calculates a 'basic atomic formula' (Phillips & Layton 1964) and classifies the analysis in accordance with the *sensu extenso* nomenclature of Phillips (1966).

If required an estimate of the iron oxidation state may be calculated for those analyses in which only total iron, as either equivalent FeO or Fe_2O_3, has been determined. The estimation is accomplished by varying the ratio $Fe^{2+}/(Fe^{2+} + Fe^{3+})$ (total iron constant) until the basic atomic formula condition

(a) $Na^A + Al^Y = Na^X + Al^Z$

is achieved. The method is only applicable to calciferous and alkali amphiboles, that is amphiboles lying within amphibole compositional space. It can be shown theoretically that the resultant range of iron oxidation states for which the basic atomic formula condition applies varies systematically over amphibole compositional space. Unfortunately, for the great majority of compositions in amphibole compositional space the range of indicated iron oxidation states is either extensive or complete, see Chapter 3. However, by applying further constraints such as (i) Si must be less than 8.08atoms, (ii) Ca in X less than 2.02atoms, (iii) sum of the A site less than 1.01atom, (iv) that the substitution $2Fe^{3+} = \square = 3Fe^{2+}$ is not applicable, in which case the amount of ferric iron concerned can be added to the sum of $Na^A + Al^Y$ and will in most cases render the two sides of condition (a) unequal, it is normally possible to restrict the iron oxidation state

affectively if this was not possible from the basic atomic formula alone.

Data Input.

Data input is in the form of PL/1 data directed statements. For each separate amphibole analysis, a title, the name and values for the oxides are input in any order. The title is in the general form

TITLE = 'Any combination of numerals or letters making up the identification of the specimen up to a maximum of 1750 characters. The title must be enclosed in quotation marks and followed by a comma. Quotation marks within the title should be avoided or if present must be doubled up i.e.''. This complete description is a valid title.',

the oxides are in the general form

oxide name = value, e.g. SIO2 = 45.67,

Each oxide is separated from the following oxides by a comma. When the last data item for each analysis is reached, a semicolon replaces the comma. Additional analyses can then follow. There is no need to mark the completion of the data

e.g. TITLE = 'AMPHIBOLE TAKEN FROM BLOGGS (1980), THERE ARE CALCITE IMPURITIES REPORTED.', SIO2=56.78, AL203 = 23.0956, FEO=6.89, -----F=2.5; SIO2 = 45.89, A1203 = 0.09, TITLE = '567', FEO= 5.34, ------ ;

Data input is restricted to the following oxides in the present implementation of MINDATA5,

SIO2., P205 , A1203 , CR203 , FE203 , V203 , FEO , MNO , ZNO , COO , NIO , MGO , LI2O , ZRO2 , TIO2 , CAO , BAO , SRO , NA2O , K2O , H2OP , H2OM , F , CL , CO2 , S , CUO , CDO , PBO , BEO , B203.

Oxides of additional elements or differing oxides of the above elements will not be included in the calculation of the atomic formula and any of the processing. Attention is drawn to the symbols used for water, H2OP and H2OM for H_2O^+ and H_2O^- respectively. The analytical total can be input as TOTAL.

The above description refers to analyses in which no estimates of the iron oxidation state is to be undertaken. If an estimate is required the process is initiated by the command

PROBE = 'YES',

This must be included with the data for each analysis for which an estimate is required. The default is not to make an estimate. This can be followed by further optional parameters which define the limits of the iron oxidation state to be investigated and the increment size used. These parameters are in terms of the reduced iron ratio (Fe^{2+} x 100) / (Fe^{2+} + Fe^{3+}) see Chapter 3. Hence the value 100 is all iron as FeO and 0 all iron as Fe_2O_3. Three parameters are used

LBOUND = value, UPBOUND = value, STEP = value,

referring to the lower limit (most oxidised), upper limit (most reduced) and the increment size respectively. The paramaters default to LBOUND = 20, UPBOUND = 100, STEP = 10. For most purposes the best choice of conditions has been found to be LBOUND = 20, UPBOUND = 95, (because UPBOUND = 100 is the same as the 23 oxygen atomic formula if all iron was quoted as FeO initially) and STEP = 10.

example of input

PROBE = 'YES', LBOUND = 30, UPBOUND = 95, STEP = 5, TITLE = 'IRON OXIDATION ESTIMATION',

SIO2 = 56.78, AL2O3 = 3.0, FEO = 24.97, - - - - - - ;

Implementation.

Program MINDATA5 requires two external PL/1 subroutines

to be compiled separately and linked at execution. The subroutines are entitled AXYZ and ATOMIC, and are listed below.

Table A4.1. Listing of program MIDAT A5.

```
MINDATA:PROC OPTIONS (MAIN);

/*    PL/1        */

/*  J.L.KNIGHT   1972    */

/* MINDATA5          */

/* REQUIRES EXTERNAL SUBROUTINES   AXYZ, ATOMIC, */

/* PROGRAM TO RECALCULATE AN ATOMIC FORMULA OF AN AMPHIBOLE
FROM A CHEMICAL ANALYSIS TO THE ANION BASE OF 24 OXYGENS AND 23
OXYGENS                                                        */

/* IN ADDITION CALCULATES A  BASIC ATOMIC FORMULA  (PHILLIPS AND
LAYTON 1964) AND NAMES THE ANALYSIS IN ACCORDANCE WITH THE S.E.
NOMENCLATURE OF PHILLIPS(1966).                                */

/* IF REQUIRED AN OPTIMUM IRON OXIDATION STATE IS CALCULATED FOR
 ANALYSES WITH EITHER ALL IRON QUCTED AS EQUIVALENT FEO OR FE203.
 THE PROCESS OF OPTIMISATION IS ACCOMPLISHED BY VARYING THE FEO/FE203 RATIO
 (TOTAL IRON CONSTANT) UNTIL THE BASIC ATOMIC FORMULA CONDITION

                    ( A + Y ) = ( X + Z )

                                          IS ACHIEVED.
 THE OPTIMISATION PROCESS FOR EACH ANALYSIS IS INITIATED BY THE
COMMAND
```

```
          PROBE='YES',

 OPTIONAL COMANDS DEFINE THE EXTREMITIES OF THE FEO/FE2O3 RATIO INVESTIGATED
 AND THE INCREMENT STEP SIZE. ALL THESE ARE QUOTED AS PERCENTAGE FEO OF
THE TOTAL IRON AS FEO.

LBOUND=NN, UPBOUND=NN, STEP= NN,

 THESE VALUES DEFAULT TO

LBOUND=20,  UPBOUND=100,  STEP=10,

THE DEFAULT FOR PROBE IS A BLANK IN WHICH CASE THE IRON OPTIMISATION
 IS NOT PERFORMED          */


        DCL (SIO2,P2O5,AL2O3,FE2O3,CR2O3,V2O3,FEO,MNO,ZNO,COO,NIO,MGO,
             LI2O,ZRO2,TIO2,CAO,BAO,SRO,NA2O,K2O,H2OP,H2OM,F,CL,
           CUO,CDO,BEO,B2O3,PBO,
             CO2,S,TOTAL,LESS,TOTAL2,BIG(3))FLOAT,
             TITLE CHAR (1750) VAR,
             BIGNAME(3) CHAR (8) VAR;
DCL       1 OX(31) EXTERNAL,
            2 NAME CHAR (8) VAR INIT ('SIO2','P2O5','AL2O3','FE2O3',
                 'CR2O3','V2O3','FEO','MNO','ZNO','COO','NIO','MGO',
                 'LI2O','ZRO2','TIO2','CAO','BAO','SRO','NA2O',
           'K2O','H2O+','H2O-','F','CL','CO2','S','CUO','CDO','PBO',
           'BEO','B2O3'),
            2 TEST FIXED,
            2 VALENCY FIXED INIT (4,5,3,3,3,3,(6)2,1,4,4,(3)2,(4)1,
           -1,-1,0,0,2,2,2,2,3),
            2 WTPC FLOAT,
            2 PLACES FIXED,
            2 MOLWT   FLOAT          INIT (60.09,141.95,101.96,159.70,
```

```
                        152.02,149.90,71.85,70.94,81.38,74.94,74.71,
                        40.32,29.88,123.22,79.90,56.08,153.36,103.63,
                        61.982,94.20,18.016,18.016,19.00,35.457,
          44.011,32.066,79.539,156.119,223.189,25.012,69.619),
           (2 MOLPROP,
            2 OXYGENS,
            2 CATS,
            2 CAT23,
            2 CAT24) FLOAT,
            2 CATNAME CHAR (8) VAR INIT ('SI','P','AL','FEIC','CR',
                        'V','FEOUS','MN','ZN','CO','NI',
                        'MG','LI','ZR','TI','CA','BA','SR','NA','K',
        'H','H-','F','CL','CO2','S','CU','CD','PB','BE','B');
DCL (
   (OH(0:4),Z(0:5),YZX(0:6),Y(0:13),X(0:11),AX(0:4),A(0:7))
FLOAT, J FIXED BIN,RR(12) FIXED BIN) EXTERNAL;
DCL
FIGS ENTRY(FLOAT) RETURNS(FIXED BIN),
       N FIXED BIN,
            P FIXED,
           (OXTOT,FAC23,FAC24,VALCK23,VALCK24) FLOAT,
           (CHECKTOT,CHECKTOT2) FLOAT,
(LAB(3),ERR(28)) LABEL;
DCL AXYZ ENTRY(FLOAT);
DCL ATOMIC ENTRY(FLOAT);
       DCL   (CONDA,CONDB,CONDC,CONDD) BIT(1);
DCL (BASIC(6),TOBAL) FLOAT;
DCL (INK,NY) FLOAT, OSIGN FIXED BIN, PROBE CHAR(3);
FIGS:PROC(NUMB)   RETURNS(FIXED BIN);
 DCL NUMB FLOAT;
 IF TRUNC((1000*NUMB)-10*TRUNC(100*NUMB))=0 THEN
            RETURN (2); ELSE RETURN (3);
        END FIGS;
ON ENDFILE(SCARDS) GOTO FINISH;
DCL (UPBOUND,STEP) FIXED BIN;
```

```
          START:SIO2,P2O5,AL2O3,FE2O3,CR2O3,V2O3,FEO,MNO,ZNO,COO,
                NIO,MGO,LI2O,ZRO2,TIO2,CAO,BAO,SRO,NA2O,K2O,H2OP,H2OM,
           F,CL,CO2,S,TOTAL,LESS,TOTAL2,CUO,CDO,PBO,BEO,B2O3 = -1;
ERR(4) = START;
       NOCYCLE = 0;
PROBE = ' ';
OXY=23; EZK=0;
INK=100;
LBOUND=20;UPBOUND=100;STEP=10;
     D2: DO N=1 BY 1 TO 31;
                 OX(N).TEST,OX(N).WTPC,OX(N).MOLPROP,OX(N).OXYGENS,
                 OX(N).CATS=0;
             END D2;
              PUT PAGE;
              GET COPY DATA;
              OX(1).WTPC=SIO2;OX(2).WTPC=P2O5;OX(3).WTPC=AL2O3;
              OX(4).WTPC=FE2O3;OX(5).WTPC=CR2O3;OX(6).WTPC=V2O3;
              OX(7).WTPC=FEO;OX(8).WTPC=MNO;OX(9).WTPC=ZNO;
              OX(10).WTPC=COO;OX(11).WTPC=NIO;OX(12).WTPC=MGO;
              OX(13).WTPC=LI2O;OX(14).WTPC=ZRO2;OX(15).WTPC=TIO2;
              OX(16).WTPC=CAO;OX(17).WTPC=BAO;OX(18).WTPC=SRO;
              OX(19).WTPC=NA2O;OX(20).WTPC=K2O;OX(21).WTPC=H2OP;
              OX(22).WTPC=H2OM;OX(23).WTPC=F;OX(24).WTPC=CL;
          OX(25).WTPC =CO2;OX(26).WTPC=S;
          OX(27).WTPC=CUO;OX(28).WTPC=CDO;OX(29).WTPC=PBO;
          OX(30).WTPC=BEO;OX(31).WTPC=B2O3;
BEGIN:ERR(1),ERR(2),ERR(3) = BLANK;
D1:  DO N = 5 TO 28;
ERR(N) = NIL;
END D1;
D3: DO N = 1 TO 31;
             IF OX(N).WTPC=-1 THEN
           D4:DO;  OX(N).TEST=-1;
                   OX(N).WTPC=0 ;
           END D4;
```

```
            END D3;
             CHECKTOT=SUM(OX.WTPC);
             CHECKTOT2=CHECKTOT;
             CHECKTOT=CHECKTOT-TOTAL;
            IF ABS(CHECKTOT)>0.01 THEN ERR(1)=ERP1;
             CHECKTOT=CHECKTOT2;
             IF OX(23).WTPC>0 THEN
             CHECKTOT2=CHECKTOT2-8*OX(23).WTPC/OX(23).MOLWT;
             IF OX(24).WTPC>0 THEN
             CHECKTOT2=CHECKTOT2-8*OX(24).WTPC/OX(24).MOLWT;
            IF LESS=-1 & (OX(23).WTPC>0 | OX(24).WTPC>0) THEN
          D5:DO;  TOTAL2=CHECKTOT2; LESS=CHECKTOT-CHECKTOT2;
            END D5; ELSE
            IF LESS=-1 THEN GO TO SEEK;
            IF ABS(TOTAL2-CHECKTOT2)>0.01 THEN ERR(2)=ERP2;
       SEEK:BIG(1),BIG(2),BIG(3)=0;
             BIG(1)=OX(1).WTPC; BIGNAME(1)=OX(1).NAME;
    D6:  DO N=2 BY 1 TO 31;
            IF OX(N).WTPC>BIG(1) THEN
          D7:DO;  BIG(3)=BIG(2); BIGNAME(3)=BIGNAME(2);
                  BIG(2)=BIG(1); BIGNAME(2)=BIGNAME(1);
                  BIG(1)=OX(N).WTPC;  BIGNAME(1)=OX(N).NAME;
            END D7; ELSE
            IF OX(N).WTPC>BIG(2) THEN
          D8:DO;  BIG(3)=BIG(2); BIGNAME(3)=BIGNAME(2);
                  BIG(2)=OX(N).WTPC;  BIGNAME(2)=OX(N).NAME;
            END D8; ELSE
            IF OX(N).WTPC>BIG(3) THEN
     D9:DO; BIG(3)=OX(N).WTPC;  BIGNAME(3)=OX(N).NAME;
      END D6;
      D10:DO N=1 TO 3;
        IF FIGS(BIG(N))=2 THEN LAB(N)=F2;  ELSE LAB(N)=F3;
     END D10;
D11:CALC:DO N=1 BY 1 TO 31;
            IF FIGS(OX(N).WTPC)=2 THEN
```

```
                OX(N).PLACES=2; ELSE OX(N).PLACES=3;
                OX(N).MOLPROP=OX(N).WTPC/OX(N).MOLWT;
               IF OX(N).VALENCY=1 | OX(N).VALENCY=2 THEN
                  OX(N).OXYGENS=OX(N).MOLPROP; ELSE
               IF OX(N).VALENCY=3 THEN
                  OX(N).OXYGENS=OX(N).MOLPROP*3; ELSE
               IF OX(N).VALENCY=4 THEN
                  OX(N).OXYGENS=OX(N).MOLPROP*2; ELSE
               IF OX(N).VALENCY=5 THEN
                  OX(N).OXYGENS=OX(N).MOLPROP*5; ELSE
               IF OX(N).VALENCY=-1 THEN
                  OX(N).OXYGENS=OX(N).MOLPROP/2;
               END CALC;
                OXTOT=0;
D12:      DO N=1 BY 1 TO 21,23,24,25,26,27,28,29,30,31;
                OXTOT=OXTOT+OX(N).OXYGENS;
               END D12;
                FAC24=24/OXTOT;
 FAC23= OXY/(OXTOT-OX(21).OXYGENS-OX(23).OXYGENS-
                          OX(24).OXYGENS);
                VALCK23,VALCK24=0;
D13:      DO N=1 BY 1 TO 21,23,24,25,26,27,28,29,30,31;
               IF OX(N).VALENCY=1 | OX(N).VALENCY=3 | OX(N).VALENCY=5
                THEN OX(N).CATS=OX(N).MOLPROP*2; ELSE
               IF OX(N).VALENCY=2 | OX(N).VALENCY=4 | OX(N).VALENCY=-1
                THEN OX(N).CATS=OX(N).MOLPROP;
                OX(N).CAT23=OX(N).CATS*FAC23;
                OX(N).CAT24=OX(N).CATS*FAC24;
                VALCK23=VALCK23+OX(N).CAT23*ABS(OX(N).VALENCY);
                VALCK24=VALCK24+(OX(N).CAT24*ABS(OX(N).VALENCY));
              END D13;
D131:   DO N=21,23,24,25,26,27,28,29,30,31;
                VALCK23=VALCK23-OX(N).CAT23*ABS(OX(N).VALENCY);
                END D131;
                VALCK23=VALCK23-46;
```

```
                VALCK24=VALCK24-48;
               IF ABS(VALCK23)<0.005 THEN VALCK23=0;
               IF ABS(VALCK24)<0.005 THEN VALCK24=0;
IF VALCHK23 > 0.0 THEN ERR(7) = ERP7;
IF VALCHK24 > 0.0 THEN ERR(8) = ERP8;
IF OX(25).WTPC>0 THEN ERR(9) = ERP9;
IF OX(26).WTPC>0 THEN ERR(10) = ERP10;
IF NOCYCLE > 0 THEN DO;
DO N = 1 TO 21,23,24,25,26,27,28,29,30,31;
OX(N).CAT24=OX(N).CAT23;
END;
GOTO N7;
END;
ATFORM24:  OH,AX =0;YZX =0;Y = 0;X =0; Z =0;A = 0;
               /* OH GROUP */
       /*CL*/
               IF OX(24).CAT24<0.01 THEN GO TO N1;
               IF OX(24).CAT24¬>0.10 & OX(23).CAT24>0.10 THEN
          D18:DO;
                OH(2)=OH(2)+OX(24).CAT24;
                OH(0)=OH(0)+OX(24).CAT24;
                OH(1)=-1;
                GO TO N3;
               END D18;
               IF OX(24).CAT24¬>0.10 & OX(23).CAT24¬>0.10 THEN
          D19:DO;
                OH(3)=OH(3)+OX(24).CAT24;
                OH(0)=OH(0)+OX(24).CAT24;
                OH(1)=-1;
                GO TO N2;
               END D19;
               IF OX(24).CAT24>0.10 THEN
          D20:DO;
                OH(1)=OX(24).CAT24;
                OH(0)=OH(0)+OH(1);
```

```
                END D20;
/* F */       N1:IF OX(23).CAT24<0.01 THEN
                   GO TO N4;
                  IF OX(23).CAT24¬=>0.10 & OX(24).CAT24>0.10 THEN
              D21:DO;
                   OH(1)=OH(1)+OX(23).CAT24;
                   OH(0)=OH(0)+OX(23).CAT24;
                   OH(2)=-1;
                   GO TO N4;
                  END D21;
                  IF OX(23).CAT24¬=>0.10 & OX(24).CAT24¬=>0.10 THEN
         N2:D22:DO;
                   OH(3)=OH(3)+OX(23).CAT24;
              OH(0)=OH(0)+OX(23).CAT24;
                   OH(2)=-1;
                   GO TO N4;
                  END D22;
                  IF OX(23).CAT24>0.10 THEN
         N3:D23:DO;
                   OH(2)=OH(2)+OX(23).CAT24;
                   OH(0)=OH(0)+OX(23).CAT24;
                  END D23;
               N4:ERR(4)=START;
/* OH */          IF OH(0)>2.02 THEN
            D231:DO;
ERR(11) = ERP11;
                   ERR(4)=ATFORM23;
                  END D231;
                  IF OH(0)+OX(21).CAT24>3.03 THEN
            D232:DO;
ERR(12) = ERP12;
                   ERR(4)=ATFORM23;
                  END D232;
                  IF OX(21).TEST=-1 & OH(0)=0 THEN
            D233:DO;
```

```
ERR(13) = ERP13;
          ERR(4)=ATFORM23;
         END D233;
       N5:IF OX(21).CAT24<0.01 THEN
          GO TO N6; ELSE
         IF OX(21).CAT24¬>0.10 THEN
      D24:DO;
         IF OH(0)>0.10 THEN
      D25:DO;
         IF OH(1)>0.01 & OH(1)>OH(2) THEN
      D26:DO;
          OH(1)=OH(1)+OX(21).CAT24;
     OH(0)=OH(0)+OX(21).CAT24;
          OH(3)=-1;
          GO TO N6;
         END D26; ELSE
         IF OH(2)>0.01 THEN
      D27:DO;
          OH(2)=OH(2)+OX(21).CAT24;
     OH(0)=OH(0)+OX(21).CAT24;
          OH(3)=-1;
          GO TO N6;
         END D27; ELSE;
      D28:DO;
          OH(3)=OH(3)+OX(21).CAT24;
          OH(0)=OH(0)+OX(21).CAT24;
          GO TO N6;
         END D24; ELSE
      D29:DO;
         IF OH(0)+OX(21).CAT24¬>2.00 THEN
      D30:DO;
          OH(3)=OH(3)+OX(21).CAT24;
          OH(0)=OH(0)+OX(21).CAT24;
          IF ROUND(OH(0),2)=2.00 THEN
          GO TO N7;
```

```
                GO TO N6;
               END D30; ELSE
            D31:DO;
/* XS H */ IF OH(0) > 2.00 THEN
D311: DO;
 OH(3)=0;
A(3)=OX(21).CAT24;
A(0)=A(0)+0.5*A(3);
ERR(4)=ATFORM23;
GOTO N7;
END D311;
OH(0)=2-OH(0);
OH(3)=OH(3)+OH(0);
A(3)=OX(21).CAT24 -OH(0);
A(0)=A(0)+0.5*A(3);
OH(0)=2;
                ERR(4)=ATFORM23;
                GO TO N7;
END D31;
               END D29;
/*OXY */    N6:IF OH(0)<2.00 & 2-OH(0)¬>OX(4).CAT24 THEN
           D32:DO;
               OH(4)=2-OH(0);
               OH(0)=2;
               Y(3)=OH(4); Y(0)=Y(0)+Y(3);
               ERR(4)=ATFORM23;
               GO TO N7;
              END D32;
ERR(14) = ERP14;
               ERR(4)=ATFORM23;
/*Z GROUP */
   /* SI */N7:
IF OXY>23 & EZK=1 THEN DO;
IF OX(4).CAT24>2.0*(OXY-23)        THEN Y(3)=2.0*(OXY-23);
ELSE Y(3)=OX(4).CAT24;
```

```
Y(0)=Y(0)+Y(3);
END;
IF OXY<23 & EZK=1 THEN DO; A(3)=A(3)+2.0*(23-OXY);
A(0)=A(0)+(23-OXY); END;
IF OX(2).CAT24> 0.008 THEN ERR(15) = ERP15;
IF OX(1).CAT24> 8.08 THEN ERR(16) = ERP16;
CALL AXYZ(DUMMY);
IF RR(1)=1 THEN ERR(17)=ERP17;
IF RR(2)=1 THEN ERR(18)=ERP18;
IF RR(3)=1 THEN ERR(19)=ERP19;
IF RR(4)=1 THEN ERR(20)=ERP20;
IF RR(5)=1 THEN ERR(21)=ERP21;
IF RR(6)=1 THEN ERR(22)=ERP22;
IF RR(7)=1 THEN ERR(23)=ERP23;
IF RR(8)=1 THEN ERR(24)=ERP24;
IF RR(9)=1 THEN ERR(25)=ERP25;
IF RR(10)=1 THEN ERR(26)=ERP26;
IF RR(11)=1 THEN ERR(27)=ERP27;
IF RR(12)=1 THEN ERR(28)=ERP28;
IF NOCYCLE = 0 THEN GOTO OUTPUT;
    ELSE GOTO SHORT;
/* OUTPUT SEGMENT */
OUTPUT: IF EZK=1 THEN GOTO G1;
PUT EDIT('R.P. MINDATA MOD.5 J.L.K. 1.5.72',DATE)
        (PAGE,A,COL(100),A)
              (BIGNAME(1),BIG(1))(LINE(2),COL(50),A,X(2),R(LAB(1)));
      PUT EDIT (BIGNAME(2),BIG(2))(X(2),A,X(2),R(LAB(2)));
              PUT EDIT(BIGNAME(3),BIG(3))(X(2),A,X(2),R(LAB(3)));
              PUT SKIP(2);
              PUT EDIT(TITLE)(SKIP,A);
              PUT SKIP(2);
              PUT EDIT ('OXIDE','WT.PC','MOLPROP','CATS/23','CATS/24')
         (A,X(7),A,X(7),A,X(4),A,X(4),A);
           F1:FORMAT (F(6,4));
           F2:FORMAT (F(6,2),X(1));
```

```
            F3:FORMAT (F(7,3));
               PUT SKIP(1);
D14:        DO N=1 BY 1 TO 31;
               IF OX(N).TEST=0 THEN
             D15:DO;
               IF OX(N).PLACES=2 THEN LAB(1)=F2; ELSE LAB(1)=F3;
                PUT EDIT(OX(N).NAME,OX(N).WTPC,OX(N).MOLPROP,
                         OX(N).CAT23,OX(N).CAT24)
                (SKIP,A(8),X(3),R(LAB(1)),X(7),R(F1),X(4),R(F3),X(5),
                 R(F3));
               END D14;
                IF FIGS(TOTAL)=2 THEN
                LAB(1)=F2; ELSE
                LAB(1)=F3;
                PUT EDIT ('TOTAL',TOTAL)(SKIP,A(8),X(3),R(LAB(1)));
                IF LESS>0 THEN
             D151:DO;
                IF FIGS(LESS)=2 THEN LAB(1)=F2;ELSE LAB(1)=F3;
                PUT EDIT('O=F,CL',LESS)(SKIP,A(8),X(3),R(LAB(1)));
                IF FIGS(TOTAL2)=2 THEN LAB(1)=F2;ELSE LAB(1)=F3;
                PUT EDIT('TOTAL',TOTAL2)(SKIP,A(8),X(3),R(LAB(1)));
               END D151; ELSE
PUT SKIP;
PUT EDIT('FACT/23',FAC23,'FACT/24',FAC24)(COL(30),A,F(6,3),X(2),A,
        F(6,3));
GOTO G1;
SHORT: PUT SKIP(2);
PUT EDIT('- - - - - - - - - - - - - - - - - - - - - - - - - -')
(COL(10),A);
PUT SKIP(2);
PUT EDIT('CYCLE',NOCYCLE,'FE2O3',OX(4).WTPC,'FEO',OX(7).WTPC,
'FE2 * 100 / FE2 + FE3',INK)(COL(20),A,F(5),X(2),A,F(8,3),X(2),
A,F(8,3),X(2),A,F(6,1));
JJ=1;
GOTO G2;
```

```
G1: PUT SKIP(5);
 JJ=0;
DO N=1 TO 3;
GOTO ERR(N);
ERP1: PUT EDIT('ERROR IN TOTAL')(R(W1));
GOTO BLANK;
ERP2: PUT EDIT('ERROR IN O=F,CL OR TOTAL2')(R(W1));
BLANK: END;
G2:
PUT SKIP;
PUT EDIT('WARNINGS RAISED DURING ELEMENT ALLOCATION TO ATOMIC FORMULA')
        (COL(5),A);
PUT SKIP(2);
KOUNT = 0;
DO N = 7 TO 28;
GOTO ERR(N);
ERP7: PUT EDIT('VALENCY CHECK 23 = ',VALCHK23)(R(W2));      GOTO G103;
ERP8: PUT EDIT('VALENCY CHECK 24 = ',VALCHK24)(R(W2));     GOTO G103;
ERP9: PUT EDIT('CARBONATE IMPURITY')(R(W1));               GOTO G103;
ERP10: PUT EDIT('SULPHIDE IMPURITY')(R(W1));               GOTO G103;
ERP11: PUT EDIT('F+CL GREATER THAN 2.02')(R(W1));          GOTO G103;
ERP12: PUT EDIT('F+CL+OH GREATER THAN 3.03')(R(W1));       GOTO G103;
ERP13: IF JJ=0 THEN
PUT EDIT('NO H2O+,F OR CL IN ANALYSIS')(R(W1)); GOTO G103;
ERP14: IF JJ=0 THEN
PUT EDIT('OXY NOT BALANCED BY FEIC')(R(W1)); GOTO G103;
ERP15: PUT EDIT('P2O5 NOT INCLUDED IN CALCULATION')(R(W1)); GOTO G103;
ERP16: PUT EDIT('SI GREATER THAN 8.08')(R(W1));            GOTO G103;
ERP17: PUT EDIT('SI + BE + B + AL LESS THAN 7.95')(R(W1)); GOTO G103;
ERP18: PUT EDIT('SI + BE GREATER THAN 8.08 CHECK')(R(W1));
GOTO G103;
ERP19: PUT EDIT('SI + BE + B GREATER THAN 8.08 CHECK')(R(W1));
GOTO G103;
ERP20: PUT EDIT('ERROR IN OH GROUP TOTAL CHECK')(R(W1));  GOTO G103;
ERP21: PUT EDIT('ERROR IN Z GROUP TOTAL')(R(W1));         GOTO G103;
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ERP22: PUT EDIT('ERROR IN YZX GROUP TOTAL')(R(W1));          GOTO G103;
ERP23: PUT EDIT('ERROR IN Y GROUP TOTAL')(R(W1));            GOTO G103;
ERP24: PUT EDIT('ERROR IN LI MN CO FEOUS MG TO X')(R(W1));
GOTO G103;
ERP25: PUT EDIT('LI UNSATISFACTORY')(R(W1));                 GOTO G103;
ERP26: PUT EDIT('ERROR IN COMPLETING Y')(R(W1));             GOTO G103;
ERP27: PUT EDIT('HIGH BA+SR INCLUDED WITH CA')(R(W1));       GOTO G103;
ERP28: PUT EDIT('X VACANCIES')(R(W1));                       GOTO G103;
NIL:  KOUNT = KOUNT + 1;
G103: END;
IF KOUNT = 22 THEN
PUT EDIT('NONE')(R(W1));
W1: FORMAT(COL(2),A);
W2: FORMAT(COL(2),A,F(6,4));
PUT SKIP;
PUT EDIT('ATOMIC FORMULA')(COL(45),A);
                PUT SKIP(2);
PUT EDIT('A  SITE')(COL(5),A,SKIP(2));
PUT SKIP;
DUMMY=0;
CALL ATOMIC(DUMMY);
PUT SKIP(2);
IF JJ=1 THEN GOTO G3;
PUT EDIT('AMPHIBOLE TYPE:  BASED OPON THE SUM OF THE Y SITE AND X SITE
OCCUPANCY')(COL(5),A,SKIP(2));
PUT SKIP(2);
                IF J=1 THEN
                PUT LIST ('  ORTHORHOMBIC - SUSPECT ANALYSIS');
                ELSE IF J=2 THEN
                PUT LIST ('  ORTHORHOMBIC');
                ELSE IF J=3 THEN
                PUT LIST ('  LIME POOR');
                ELSE IF J=4 THEN
                PUT LIST ('  HIGH/LOW LIME HYBRID');
                ELSE IF J=5 THEN
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                PUT LIST ('  HIGH/LOW LIME HYBRID');
                ELSE IF J=6 & X(2)<=1.00 THEN
                PUT LIST ('  CALCIFEROUS');
                ELSE IF J=6 & X(2)>1.00  THEN
                PUT LIST ('  ALKALI');
                PUT SKIP(2);
PUT EDIT('BASIC FORMULA:  ELEMENTS OTHER THAN CA MG, SI CONVERTED TO EQU
IVALENT NA OR AL')(COL(5),A,SKIP(2));
PUT SKIP(2);
 G3:
/*  BESI = 2AL */
G100: Z(4)=Z(4)+Z(4);
BASIC(1)=A(0)+A(4)+A(6)+A(7)+AX(0)+AX(4)+0.5*A(3);
BASIC(2)= X(1)+X(3)+X(4)+X(5)+X(7)+X(8)+X(9)+X(10)+X(11);
BASIC(3)=X(2)+X(6);
BASIC(4)=Y(0)-YZX(5)-YZX(6);
BASIC(5)=YZX(0)+YZX(5)+YZX(6);
BASIC(6)=Z(3)+Z(4)+Z(5);
NY = BASIC(1)+BASIC(5)- BASIC(3) - BASIC(6);
PUT EDIT('NA',BASIC(1),'CA',BASIC(2),'NA',BASIC(3),'MG',BASIC(4);
'AL',BASIC(5),'SI',Z(1),'AL',BASIC(6))
                        (X(2),A(3),F(5,3))('022')(X(2),A(3))
                        ('OH',OH(0))(X(2),A(3),F(5,2));
                PUT LIST ('CO-ORDINATES') SKIP(2);
PUT EDIT('A=',BASIC(1),'X=',BASIC(3),'Y=',BASIC(5),'Z=',BASIC(6))
                        (X(2),A(3),F(5,3))
('A+Y=',BASIC(1)+BASIC(5),'X+Z=',BASIC(3)+BASIC(6))
(X(3),A(5),F(5,3))('A+Y-X+Z=',NY)(X(2),A(8),F(7,3));
                PUT SKIP(2);
IF JJ=1 THEN DO;
IF NY>0.2 & OXY=23 THEN GOTO START;
WATER=(24.0*(OXTOT-OX(21).OXYGENS-OX(23).OXYGENS-OX(24).OXYGENS)
/ 23.0) -(OXTOT-OX(21).OXYGENS-OX(23).OXYGENS-OX(24).OXYGENS);
WATER=WATER * 18.0;
PUT EDIT('CALC. WATER CONTENT',WATER)( COL(40),A,X(2),F(6,3));
```

```
X(2)=X(2)+X(6);
Z(3)=Z(3)+Z(4)+Z(5);
Y(0)=YZX(0)+YZX(5)+YZX(6);
GOTO G4; END;
IF BASIC(3)+BASIC(6)-BASIC(5)> 1.00 | BASIC(3)+BASIC(6)-BASIC(5) < 0.0
THEN
                PUT LIST ('GENERAL CONDITION X-Y+Z=0 TO 1 NOT SATISFIED'
                );
IF ABS(BASIC(1)+BASIC(5)-BASIC(3)-BASIC(6))> 0.02 THEN
PUT LIST('A+Y NOT EQUAL TO X+Z');
A(0) = A(0)+A(4)+A(6)+A(7)+AX(0)+AX(4)+0.5*A(3);
                PUT SKIP(2);
                PUT LIST('K/NA IN A BASIC=');
                IF A(0)>0 THEN
                PUT EDIT((A(2)+AX(2))/A(0))(F(8,3)); ELSE
                PUT LIST('NOT CALC');
                PUT LIST('FEUS IN Y/MG IN Y BASIC=');
                IF Y(0)<5.00 THEN
                PUT EDIT(Y(2)/(Y(0)-YZX(5)-YZX(6)))(F(8,3)); ELSE
                PUT LIST('NOT CALC');
                PUT SKIP;
PUT LIST('FEUS X+Y/MG+CA BASIC=');
                IF X(2)<2.00 THEN
PUT EDIT((Y(2)+X(5))/(Y(0)-YZX(5)-YZX(6)+X(1)+X(3)+X(4)+X(5)+X(7)+X(8)+
X(9)+X(10)+X(11)))(F(8,3)); ELSE
                PUT LIST('NOT CALC');
                PUT LIST('FEIC YZX/AL Y BASIC=');
                IF YZX(0)>0 THEN
                PUT EDIT(YZX(2)/(YZX(0)+YZX(5)+YZX(6)))(F(8,3)); ELSE
                PUT LIST('NOT CALC');
                PUT SKIP;
                PUT LIST('FEIC YZX/FE TOTAL=');
                IF Y(2)+Y(3)+YZX(2)+X(5)+Y(12)>0 THEN
                PUT EDIT(YZX(2)/(Y(2)+Y(3)+Y(10)+Y(12)+YZX(2)+X(5)))
                (F(8,3)); ELSE PUT LIST('NOT CALC');
```

```
                PUT LIST('FEIC TOTAL/FE TOTAL=');
                IF Y(2)+Y(3)+YZX(2)+X(5)+Y( 2)>0 THEN
                PUT EDIT((YZX(2)+Y(3)+Y(10)+Y(12))/(YZX(2)+Y(3)+Y(10)
                +Y(12)+Y(2)+X(5)))(F(8,3)); ELSE PUT LIST('NOT CALC');
                PUT SKIP;
                PUT LIST('2TI VAC/MG Y BASIC=');
                IF Y(0)<5.00 THEN
                PUT EDIT((2*Y(11))/(Y(0)-YZX(5)-YZX(6)))(F(8,3)); ELSE
                PUT LIST('NOT CALC');
                PUT LIST('2TI YZX/AL YZX BASIC=');
                IF YZX(0)>0 THEN
                PUT EDIT((2*YZX(6))/(YZX(0)+YZX(5)+YZX(6)))(F(8,3));
                ELSE PUT LIST('NOT CALC');
                PUT LIST('100MG/(MG+FEUS+FEIC+MN) =') SKIP;
IF OX(12).CAT24+OX(7).CAT24+OX(4).CAT24+OX(8).CAT24 > 0 THEN
                PUT EDIT(100*OX(12).CAT24/(OX(12).CAT24+OX(7).CAT24
                +OX(4).CAT24+OX(8).CAT24))(F(8,3));
ELSE PUT LIST ('NOT CALC');
X(2)= X(2)+X(6);
Z(3)=Z(3)+Z(4)+Z(5);
                Y(0)=YZX(0)+YZX(5)+YZX(6);
PUT EDIT('OBLIQUE AXES','RECTANGULAR AXES')(COL(7),A,COL(45),A);
PUT EDIT('FIRST ORIENTATION','SECOND ORIENTATION')(COL(30),A,COL(60),A)
;
PUT EDIT('X(NEW)//X =X+Y=  ',X(2)+Y(0),'X(NEW) = (X+Y)*SQRT3 = ',
(X(2)+Y(0))*SQRT(3),'X(NEW)//Y =X+2Y+Z  = ',X(2)+2*Y(0)+Z(3))
     (COL(2),A,F(6,2),COL(27),A,F(6,2),COL(58),A,F(6,2));
PUT EDIT('Y(NEW)//Z =Y+Z=  ',Y(0)+Z(3),'Y(NEW)//Z = 2+2Z+Y-X = ',
2+Y(0)-X(2)+2*Z(3), 'Y(NEW) =(2-X+Z)*SQRT3 = ',2-X(2) +Z(3)*SQRT(3))
     (COL(2),A,F(6,2),COL(27),A,F(6,2),COL(58),A,F(6,2));
                PUT LIST ('CONDITION A: Z<=Y-X+1/2: ') SKIP(3);
                IF Z(3)<=Y(0)-X(2)+1/2 THEN
PUT EDIT('  YES')(A); ELSE
PUT EDIT('  NO')(A);
                PUT LIST ('CONDITION B: Z<=X: ') SKIP;
```

```
                IF Z(3)<=X(2) THEN
                PUT LIST (' YES'); ELSE
                PUT LIST (' NO');
                PUT LIST ('CONDITION C: Z<=2-Y: ') SKIP;
                IF Z(3)<=2.00-Y(0) THEN
                PUT LIST (' YES'); ELSE
                PUT LIST (' NO');
                PUT LIST ('CONDITION D: Y<=2-X: ') SKIP;
                IF Y(0)<=2.00-X(2) THEN
                PUT LIST (' YES'); ELSE
                PUT LIST (' NO');
G4: PUT LIST('BASIC FORMULA NAME') SKIP(2);
                IF Z(3)>Y(0)-X(2)+1/2 THEN CONDA='0'B;ELSE CONDA='1'B;
                IF Z(3)>X(2)          THEN CONDB='0'B;ELSE CONDB='1'B;
                IF Z(3)>2-Y(0)        THEN CONDC='0'B;ELSE CONDC='1'B;
                IF Y(0)>2-X(2)         THEN CONDD='0'B;ELSE CONDD='1'B;
                IF J<6 THEN
                PUT LIST ('NOT CALCIFEROUS OR ALKALI - CHECK');
                IF X(2)<1.00 THEN
           D65:DO;
                PUT EDIT ('CALCIFEROUS GROUP:')(SKIP,X(10),A(19),X(2));
                IF X(2)<=0.50 THEN
           D66:DO;
                IF Y(0)<=0.50 THEN
           D67:DO;
                IF Z(3)<=0.50 THEN
           D68:DO;
                IF CONDA THEN GO TO TR;
                IF CONDB THEN GO TO R;
                GO TO ED;
               END D68;
                IF Z(3)>0.50 & CONDA THEN GO TO TR;
                GO TO ED;
               END D67;
                IF Y(0)>0.50 & Y(0)<=1.00 THEN
```

```
D69:DO;
    IF Z(3)<=0.50 THEN GO TO TR;
    IF Z(3)>0.50 & Z(3)<=1.00 THEN
D70:DO;
    IF CONDA THEN GO TO TR;
    GO TO ED;
   END D70;
    IF Z(3)>1.50 THEN GO TO PA;
    IF CONDA & CONDC THEN GO TO TR;
    IF CONDA THEN GO TO TS;
    IF CONDC THEN GO TO ED;
    GO TO PA;
   END D69;
    IF Y(0)>1.00 & Y(0)<=1.50 THEN
D71:DO;
    IF Z(3)>=0.50 & Z(3)<=1.00 THEN
D72:DO;
    IF CONDA & CONDC THEN GO TO TR;
    GO TO TS;
   END D72;
    IF Z(3)>1.00 & CONDA THEN GO TO TS;
    GO TO PA;
   END D71;
    IF Y(0)>1.50 & Y(0)<=2.00 THEN
D73:DO;
    IF Z(3)>1.00 & Z(3)<=1.50 THEN GO TO TS;
    IF Z(3)>1.50 & Z(3)<=2.00 THEN
D74:DO;
    IF CONDA THEN GO TO TS;
    IF CONDD THEN GO TO PA;
    GO TO SU;
   END D66;
    IF Y(0)<=0.50 THEN
D75:DO;
    IF Z(3)<=0.50 THEN
```

```
D76:DO;
     IF CONDA THEN GO TO TR;
     GO TO R;
    END D76;
     IF Z(3)>0.50 & Z(3)<=1.00 THEN
D77:DO;
     IF CONDB THEN GO TO R;
     GO TO ED;
    END D75;
     IF Y(0)>0.50 & Y(0)<=1.00 THEN
D78:DO;
     IF Z(3)<=0.50 THEN
D79:DO;
     IF CONDA THEN GO TO TR;
     GO TO R;
    END D79;
     IF Z(3)>0.50 & Z(3)<=1.00 THEN
D80:DO;
     IF CONDA THEN GO TO TR;
     IF CONDB THEN GO TO R;
     GO TO ED;
    END D80;
     IF Z(3)>1.00 & Z(3)<=1.50 THEN
D81:DO;
     IF CONDC THEN GO TO ED;
     GO TO PA;
    END D78;
     IF Y(0)>1.00 & Y(0)<=1.50 THEN
D82:DO;
     IF Z(3)<=0.50 THEN GO TO TR;
     IF Z(3)>0.50 & Z(3)<=1.00 THEN
D83:DO;
     IF CONDA & CONDC THEN GO TO TR;
     IF CONDA THEN GO TO TS;
     IF CONDB THEN GO TO R;
```

```
     IF CONDD THEN GO TO PA;
     GO TO SU;
    END D83;
     IF Z(3)>1.00 & Z(3)<=1.50 THEN
D84:DO;
     IF CONDA THEN GO TO TS;
     IF CONDD THEN GO TO PA;
     GO TO SU;
    END D84;
     IF Z(3)>1.50 & Z(3)<=2.00 THEN
D85:DO;
     IF CONDD THEN GO TO PA;
     GO TO SU;
    END D82;
     IF Y(0)>1.50 & Y(0)<=2.00 THEN
D86:DO;
     IF Z(3)>=0.50 & Z(3)<=1.00 THEN GO TO TS;
     IF Z(3)>1.00 & Z(3)<=2.00 & CONDA THEN GO TO TS;
     GO TO SU;
    END D65;
     PUT EDIT ('ALKALI GROUP:')(SKIP,X(10),A(19),X(2));
     IF X(2)<=1.50 THEN
D87:DO;
     IF Y(0)<=0.50 & Z(3)<=0.50 THEN GO TO R;
     IF Y(0)>0.50  & Y(0)<=1.00 THEN
D88:DO;
     IF Z(3)<=0.50 THEN
D89:DO;
     IF CONDA THEN GO TO G;
     IF CONDD THEN GO TO R;
     GO TO EC;
    END D89;
     IF Z(3)<=1.00 & CONDD THEN GO TO R;
     GO TO EC;
    END D88;
```

```
      IF Y(0)>1.00  & Y(0)<=1.50 THEN
D90:DO;
      IF Z(3)<=0.50 THEN
D91:DO;
      IF CONDA THEN GO TO G;
      GO TO EC;
     END D91;
      IF Z(3)>0.50  & Z(3)<=1.00 THEN
D92:DO;
      IF CONDA THEN GO TO G;
      IF CONDC THEN GO TO EC;
      GO TO M;
     END D92;
      IF Z(3)>1.00  & Z(3)<=1.50 THEN
D93:DO;
      IF CONDB THEN GO TO M;
      GO TO SU;
     END D90;
      IF Y(0)>1.50  & Y(0)<=2.00 THEN
D94:DO;
      IF Z(3)<=0.50 THEN GO TO G;
      IF Z(3)>0.50  & Z(3)<=1.00 THEN
D95:DO ; IF CONDA THEN GO TO G;
      GO TO M;
     END D95;
      IF Z(3)>1.00  & Z(3)<=1.50 THEN
D96:DO;
      IF CONDA THEN GO TO G;
      IF CONDB THEN GO TO M;
      GO TO SU;
     END D96;
      IF Z(3)>1.50  & Z(3)<=2.00 THEN GO TO SU;
     END D87;
      IF Y(0)>=0.50 & Y(0)<=1.00 & Z(3)<=0.50 THEN GO TO EC;
      IF Y(0)>1.00  & Y(0)<=1.50 THEN
```

```
 D97:DO;
      IF Z(3)<=0.50 THEN
 D98:DO;
      IF CONDA THEN GO TO G;
      GO TO EC;
     END D98;
      IF Z(3)>0.50  & Z(3)<=1.00 THEN
 D99:DO;
      IF CONDC THEN GO TO EC;
      GO TO M;
     END D97;
      IF Y(0)>1.50  & Y(0)<=2.00 THEN
D100:DO;
      IF Z(3)<=0.50 THEN
D101:DO;
      IF CONDA THEN GO TO G;
      IF CONDC THEN GO TO EC;
      GO TO M;
     END D101;
      IF Z(3)>0.50  & Z(3)<=1.00 THEN
D102:DO;
      IF CONDA THEN GO TO G;
      GO TO M;
     END D102;
      IF Z(3)>1.00  & Z(3)<=1.50 THEN GO TO M;
     END D100;
      PUT EDIT ('NO NAME OBTAINED - CHECK')(SKIP,X(30),A(25));
      GO TO ERR(4);
  TR:PUT EDIT ('TREMOLITE S.E.')(SKIP,X(30),A(15));
      GO TO ERR(4);
  TS:PUT EDIT ('TSCHERMAKITE S.E.')(SKIP,X(30),A(18));
      GO TO ERR(4);
   G:PUT EDIT ('GLAUCOPHANE S.E.') (SKIP,X(30),A(13));
      GO TO ERR(4);
   R:PUT EDIT ('RICHTERITE S.E.')  (SKIP,X(30),A(18));
```

```
            GO TO ERR(4);
          EC:PUT EDIT ('ECKERMANNITE S.E.')(SKIP,X(30),A(18));
            GO TO ERR(4);
           M:PUT EDIT ('MIYASHIROITE S.E.')(SKIP,X(30),A(18));
            GO TO ERR(4);
          SU:PUT EDIT ('SUNDIUSITE S.E.')  (SKIP,X(30),A(18));
            GO TO ERR(4);
          PA:PUT EDIT ('PARGASITE S.E.')   (SKIP,X(30),A(15));
            GO TO ERR(4);
          ED:PUT EDIT ('EDENITE S.E.')     (SKIP,X(30),A(15));
            GO TO ERR(4);
ATFORM23: IF PROBE¬='YES' THEN DO; ERR(4)=START;EZK=1; END;
ELSE DO; ERR(4)=RECYCLE; EZK=1; END;
OH,AX = 0;YZX = 0;Y=0;X=0;Z=0;A=0;
D103: DO N=1 TO 21,23,24,25,26,27,28,29,30,31;
OX(N).CAT24 = OX(N).CAT23;
            END D103;
             PUT SKIP(2) LIST('CALCULATION BASED ON 23 OXYGENS: ');
             PUT SKIP(0) LIST('_______________________________  ');
DO N= 5 TO 28;
ERR(N)=NIL; END;
             GO TO N7;
RECYCLE:
IF OX(7).WTPC<=0.0 &NOCYCLE>1 THEN GOTO START;
IF INK-STEP < LBOUND THEN GOTO START;
NOCYCLE = NOCYCLE +1;
OH,AX =0;YZX=0;Y=0;X=0;Z=0;A=0;
/* SPECIAL CASE 1ST TIME THROUGH */
IF NOCYCLE = 1 THEN
D601: DO;
IF OX(4).WTPC > 0 &   OX(7).WTPC <= 0 THEN
D602: DO;
OX(7).WTPC = OX(4).WTPC *      0.89355;
TEMP = OX(7).WTPC;
OX(4).WTPC = 0;
```

```
TT = OX(7).WTPC + OX(4).WTPC ; TOBAL = TOTAL;
GOTO G105;
END D602;
IF OX(4).WTPC <=0 &    OX(7).WTPC > 0 THEN
DO;
TEMP = OX(7).WTPC;
OX(4).WTPC = 0;
TT = OX(7).WTPC + OX(4).WTPC ; TOBAL = TOTAL;
END;
G105: INK=UPBOUND;
GOTO G110;
END D601;
INK = INK-STEP;
G110: T = TEMP *((100.0 - INK)/ 100.0);
OX(7).WTPC = TEMP - T;
OX(4).WTPC = T *   1.119;
DIFF = (OX(7).WTPC+ OX(4).WTPC) - TT;
TOTAL = TOBAL + DIFF;
GOTO BEGIN;
       FINISH:PUT PAGE LIST('END OF RUN');
            END MINDATA;
```

Table A4.2. Listing of subroutine ATOMIC.

```
ATOMIC:PROC(DUMMY);

/*     PL/1                */

/*    J.L.KNIGHT     1972          */

/* EXTERNAL SUBROUTINE    ATOMIC    */

/* COMPLETE ATOMIC FORMULA OUTPUT     */

/* FOR USE WITH MINDATA5          */

DCL DUMMY FLOAT;
DCL       1 OX(31) EXTERNAL,
              2 NAME CHAR (8) VAR INIT ('SIO2','P2O5','AL2O3','FE2O3',
                   'CR2O3','V2O3','FEO','MNO','ZNO','COO','NIO','MGO',
                   'LI2O','ZRO2','TIO2','CAO','BAO','SRO','NA2O',
             'K2O','H2O+','H2O-','F','CL','CO2','S','CUO','CDO','PBO',
              'BEO','B2O3'),
                2 TEST FIXED,
                2 VALENCY FIXED INIT (4,5,3,3,3,3,(6)2,1,4,4,(3)2,(4)1,
             -1,-1,0,0,2,2,2,2,3),
                2 WTPC FLOAT,
                2 PLACES FIXED,
                2 MOLWT   FLOAT          INIT (60.09,141.95,101.96,159.70,
                          152.02,149.90,71.85,70.94,81.38,74.94,74.71,
                          40.32,29.88,123.22,79.90,56.08,153.36,103.63,
                          61.982,94.20,18.016,18.016,19.00,35.457,
             44.011,32.066,79.539,156.119,223.189,25.012,69.619),
```

```
              (2 MGLPROP,
               2 OXYGENS,
               2 CATS,
               2 CAT23,
               2 CAT24) FLOAT,
               2 CATNAME CHAR (8) VAR INIT ('SI','P','AL','FEIC','CR',
                         'V','FEOUS','MN','ZN','CO','NI',
                         'MG','LI','ZR','TI','CA','BA','SR','NA','K',
          'H','H-','F','CL','CO2','S','CU','CD','PB','BE','B');
DCL (
   (OH(0:4),Z(0:5),YZX(0:6),Y(0:13),X(0:11),AX(0:4),A(0:7))
FLOAT, J FIXED BIN,RR(12) FIXED BIN) EXTERNAL;
DUMMY=1;
               IF A(0)+AX(0)<1.00 THEN
               PUT EDIT ('*',1.00-A(0)-AX(0))(A(1),F(5,2));
D641:    DO N=1 TO 7;
               IF A(N)>0 THEN
               DO;
               IF N=1 THEN PUT EDIT('NA',A(1))(R(F5));
               IF N=2 THEN PUT EDIT('K',A(2))(R(F4));
               IF N=3 THEN PUT EDIT('H',A(3))(R(F4));
               IF N=4 THEN PUT EDIT('CA',A(4))(R(F5));
IF N=5 THEN PUT EDIT ('LI',A(5))(R(F5));
IF N=6 THEN PUT EDIT ('PB',A(6))(R(F5));
IF N=7 THEN PUT EDIT ('CD',A(7))(R(F5));
              END D641;
               PUT EDIT ('A  =',A(0))(R(F6));
               PUT SKIP;
      JJ=0;
         D642:DO N=1 TO 3;
               IF AX(N)>0 THEN
               DO;
        JJ=JJ+1;
               IF N=1 THEN PUT EDIT('NA',AX(1))(R(F5));
               IF N=2 THEN PUT EDIT('K',AX(2))(R(F4));
```

```
                IF N=3 THEN PUT EDIT('H',AX(3))(R(F4));
               END D642;
IF JJ>0 THEN PUT EDIT('COMPENSATION FOR MONOVALENT IONS IN X')(X(2),A);
                PUT EDIT ('AX =',AX(0))(R(F6));
                PUT SKIP; PUT EDIT('A TOTAL=',A(0)+AX(0))(R(F8));
PUT SKIP(2);
PUT EDIT('X  SITE')(COL(5),A,SKIP(2));
PUT SKIP;
D643: DO N = 1 TO 11;
                IF X(N)>0 THEN
                DO;
                IF N=1 THEN PUT EDIT('CA',X(1))(R(F5));
                IF N=2 THEN PUT EDIT('NA',X(2))(R(F5));
                IF N=3 THEN PUT EDIT('MG',X(3))(R(F5));
                IF N=4 THEN PUT EDIT('MN',X(4))(R(F5));
                IF N=5 THEN PUT EDIT('FEUS',X(5))(R(F7));
IF N=6 THEN PUT EDIT ('LI',X(6))(R(F5));
IF N=7 THEN PUT EDIT ('PB',X(7))(R(F5));
IF N=8 THEN PUT EDIT('CD',X(8))(R(F5));
IF N=9 THEN PUT EDIT ('CO',X(9))(R(F5));
IF N=10 THEN PUT EDIT('ZN',X(10))(R(F5));
IF N=11 THEN PUT EDIT('CU',X(11))(R(F5));
               END D643;
                PUT EDIT ('X TOTAL=',X(0))(R(F8));
PUT SKIP(2);
PUT EDIT('Y  SITE')(COL(5),A,SKIP(2));
PUT SKIP;
          D644:DO N=1 TO 7;
                IF Y(N)>0 THEN
                DO;
                IF N=1 THEN PUT EDIT('MG',Y(1))(R(F5));
                IF N=2 THEN PUT EDIT('FEUS',Y(2))(R(F7));
                IF N=3 THEN PUT EDIT('FEIC(OXY)',Y(3))(X(2),A(9),F(5,2));
                IF N=4 THEN PUT EDIT('MN',Y(4))(R(F5));
                IF N=5 THEN PUT EDIT('ZN',Y(5))(R(F5));
```

```
                IF N=6 THEN PUT EDIT('CO',Y(6))(R(F5));
                IF N=7 THEN PUT EDIT('NI',Y(7))(R(F5));
               END D644;
                PUT EDIT ('Y  =',Y(0))(R(F6));
PUT SKIP;
     JJ=0;
D645:   DO N = 8 TO 13;
                IF Y(N)>0 THEN
                DO;
        JJ=JJ+1;
                IF N=8 THEN PUT EDIT('LI',Y(8))(R(F5));
                IF N=9 THEN PUT EDIT('AL=LI',Y(9))(X(2),A(5),F(5,2));
                IF N=10 THEN PUT EDIT('FEIC=LI',Y(10))(X(2),A(7),F(5,2));
                IF N=11 THEN PUT EDIT('TI=MG',Y(11),'*',Y(11))
                (X(2),A(5),F(5,2),X(2),A(1),F(5,2));
                IF N=12 THEN PUT EDIT('FEIC=MG',Y(12),'*',Y(12)/2)
                (X(2),A(7),F(5,2),X(2),A(1),F(5,2));
IF N=13 THEN PUT EDIT ('CU',Y(13))(R(F5));
               END D645;
IF JJ>0 THEN PUT EDIT (' WITHIN Y SITE COMPENSATION')(X(2),A);
                PUT SKIP;
      JJ=0;
         D646:DO N=1 TO 6;
                IF YZX(N)>0 THEN
                DO;
        JJ=JJ+1;
                IF N=1 THEN PUT EDIT('AL',YZX(1))(R(F5));
                IF N=2 THEN PUT EDIT('FEIC',YZX(2))(R(F7));
                IF N=3 THEN PUT EDIT('CR',YZX(3))(R(F5));
                IF N=4 THEN PUT EDIT('V',YZX(4))(R(F4));
                IF N=5 THEN PUT EDIT('ZR',YZX(5))(R(F5));
                IF N=6 THEN PUT EDIT('TI',YZX(6))(R(F5));
               END D646;
IF JJ>0 THEN PUT EDIT('COMPENSATION EXTERNAL TO Y')(X(2),A);
                PUT EDIT ('YZX=',YZX(0))(R(F6)); PUT SKIP;
```

```
                PUT EDIT ('Y TOTAL=',Y(0)+YZX(0))(R(F8));
PUT SKIP(2);
PUT EDIT('Z  SITE')(COL(5),A,SKIP(2));
PUT SKIP;
D647:     DO N=1 TO 5;
                IF Z(N)>0 THEN
                DO;
                IF N=1 THEN PUT EDIT('SI',Z(1))(R(F5));
                IF N=2 THEN PUT EDIT('P',Z(2))(R(F4));
                IF N=3 THEN PUT EDIT('AL',Z(3))(R(F5));
IF N=4 THEN PUT EDIT ('BE',Z(4))(R(F5));
IF N=5 THEN PUT EDIT('B',Z(5))(R(F4));
              END D647;
                PUT EDIT ('Z TOTAL=',Z(0))(R(F8));
PUT SKIP(2);
PUT EDIT('HYDROXYL SITE')(COL(5),A,SKIP(2));
PUT SKIP;
          D648:DO N=1 TO 4;
                IF OH(N)>0 THEN
                DO;
                IF N=1 THEN PUT EDIT('CL',OH(1))(R(F5));
                IF N=2 THEN PUT EDIT('F',OH(2))(R(F4));
                IF N=3 THEN PUT EDIT('OH',OH(3))(R(F5));
                IF N=4 THEN PUT EDIT('O',OH(4))(R(F4));
               END D648;
                PUT EDIT ('OH TOTAL=',OH(0))(COLUMN(90),A(9),F(5,2));
            F4:FORMAT (X(2),A(1),F(5,3));
            F5:FORMAT (X(2),A(2),F(5,3));
            F6:FORMAT (COLUMN(90),A(4),F(5,3));
            F7:FORMAT (X(2),A(4),F(5,3));
            F8:FORMAT (COLUMN(90),A(8),F(5,3));
DO N = 1 TO 4;
IF OH(N)<0.0 THEN OH(N)=0.0; END;
DO N = 1 TO 5;
IF Z(N)<0.0 THEN Z(N)=0.0; END;
```

```
DO N = 1 TO 6;
IF YZX(N)<0.0 THEN YZX(N)=0.0; END;
DO N = 1 TO 13;
IF Y(N)<0.0 THEN Y(N)=0.0; END;
DO N = 1 TO 11;
IF X(N)<0.0 THEN X(N)=0.0; END;
DO N = 1 TO 4;
IF AX(N)<0.0 THEN AX(N)=0.0;          END;
DO N = 1 TO 7;
IF A(N)<0.0 THEN A(N)=0.0; END;
RETURN;
END;
```

6

Table A4.3. Listing of subroutine AXYZ.

```
AXYZ: PROC(DUMMY);

/*     PL/1              */

/*    J.L.KNIGHT    1972          */

/*EXTERNAL SUBROUTINE  AXYZ          */

/* ELEMENT ALLOCATION TO THE A, X, Y AND Z SITES     */

/* FOR USE WITH MINDATA5          */

DCL DUMMY FLOAT;
DCL       1 OX(31) EXTERNAL,
            2 NAME CHAR (8) VAR INIT ('SIO2','P2O5','AL2O3','FE2O3',
                 'CR2O3','V2O3','FEO','MNO','ZNO','COO','NIO','MGO',
                 'LI2O','ZRO2','TIO2','CAO','BAO','SRO','NA2O',
              'K2O','H2O+','H2O-','F','CL','CO2','S','CUO','CDO','PBO',
              'BEO','B2O3'),
              2 TEST FIXED,
              2 VALENCY FIXED INIT (4,5,3,3,3,3,(6)2,1,4,4,(3)2,(4)1,
             -1,-1,0,0,2,2,2,2,3),
              2 WTPC FLOAT,
              2 PLACES FIXED,
              2 MOLWT   FLOAT         INIT (60.09,141.95,101.96,159.70,
                        152.02,149.90,71.85,70.94,81.38,74.94,74.71,
                        40.32,29.88,123.22,79.90,56.08,153.36,103.63,
                        61.982,94.20,18.016,18.016,19.00,35.457,
             44.011,32.066,79.539,156.119,223.189,25.012,69.619),
```

```
            (2 MCLPROP,
             2 OXYGENS,
             2 CATS,
             2 CAT23,
             2 CAT24) FLOAT,
             2 CATNAME CHAR (8) VAR INIT ('SI','P','AL','FEIC','CR',
                       'V','FEOUS','MN','ZN','CO','NI',
                       'MG','LI','ZR','TI','CA','BA','SR','NA','K',
          'H','H-','F','CL','CO2','S','CU','CD','PB','BE','B');
DCL (
   (OH(0:4),Z(0:5),YZX(0:6),Y(0:13),X(0:11),AX(0:4),A(0:7))
FLOAT, J FIXED BIN,RR(12) FIXED BIN) EXTERNAL;
RR=0;
             IF CX(1).CAT24>=8.00  THEN
         D33:DO;
             Z(1)=OX(1).CAT24;
             Z(0)=Z(0)+Z(1);
             YZX(1)=YZX(1)+OX(3).CAT24;
             YZX(0)=YZX(0)+OX(3).CAT24;
             GO TO N8;
            END D33;
          Z(1) = Z(1) + OX(1).CAT24;
          Z(0) = Z(0) + OX(1).CAT24;
          IF OX(30).CAT24 + OX(31).CAT24 + OX(1).CAT24 + OX(3).CAT24 <
          7.95 THEN
D4000:   DO;
RR(1)=1;
          Z(3) = Z(3) + OX(3).CAT24;
          Z(4) = Z(4) + OX(30).CAT24;
          Z(5) = Z(5) + OX(31).CAT24;
          Z(0) = Z(0) + Z(3) + Z(4) + Z(5);
          GOTO N8;
          END D4000;
/* BE */   IF OX(30).CAT24 <= 0.0 THEN GOTO G1;
          Z(4) = Z(4) + OX(30).CAT24;
```

```
          Z(0) = Z(0) + Z(4);
IF Z(0) >= 8.08 THEN RR(2)=1;
/* B*/ G1: IF OX(31).CAT24 <= 0.0 THEN GOTO G2;
          Z(5) = Z(5) + OX(31).CAT24;
          Z(0) = Z(0) + Z(5);
IF Z(0) >= 8.08 THEN RR(3)=1;
          GOTO N8;
/*AL*/G2:IF Z(0) + OX(3).CAT24 <= 8.00 THEN
  D331:   DO;
          Z(3) = Z(3) + OX(3).CAT24;
          Z(0) = Z(0) + Z(3);
          GOTO N8;
          END D331;
          Z(3) = 8.00 - Z(0);
          Z(0) = Z(0) + Z(3);
          YZX(1) = YZX(1) + OX(3).CAT24 - Z(3);
          YZX(0) = YZX(0) + YZX(1);
/* ZR */    N8:IF OX(14).CAT24<0.01 THEN GO TO N9;
              IF OX(14).CAT24<0.05 THEN
           D34:DO;
              YZX(6)=YZX(6)+OX(14).CAT24;
              YZX(0)=YZX(0)+OX(14).CAT24;
              YZX(5)=-1;
              GO TO N9;
             END D34;
              YZX(5)=OX(14).CAT24;
              YZX(0)=YZX(0)+YZX(5);
/* V */     N9:IF OX(6).CAT24<0.01 THEN GO TO N10;
              IF OX(6).CAT24<0.10 THEN
           D35:DO;
              YZX(2)=YZX(2)+OX(6).CAT24;
              YZX(0)=YZX(0)+OX(6).CAT24;
              YZX(4)=-1;
              GO TO N10;
             END D35;
```

```
                YZX(4)=OX(6).CAT24;
                YZX(0)=YZX(0)+OX(6).CAT24;
/* CR */    N10:IF OX(5).CAT24<0.01 THEN GO TO N11;
                IF OX(5).CAT24<0.10 THEN
            D36:DO;
                YZX(3)=-1;
                YZX(2)=YZX(2)+OX(5).CAT24;
                YZX(0)=YZX(0)+OX(5).CAT24;
                GO TO N11;
               END D36;
                YZX(3)=OX(5).CAT24;
                YZX(0)=YZX(0)+CX(5).CAT24;
/*FEIC*/    N11:IF Y(3)>0 THEN
            D37:DO;
                YZX(2)=YZX(2)+OX(4).CAT24-Y(3);
                IF YZX(2)<0.01 THEN
            D38:DO;
                YZX(2)=0;
                GO TO N12;
               END D38;
                IF YZX(2)<0.10 THEN
            D39:DO;
                YZX(1)=YZX(1)+YZX(2);
                YZX(0)=YZX(0)+OX(4).CAT24-Y(3);
                YZX(2)=-1; GO TO N12;
               END D39;
                YZX(0)=YZX(0)+OX(4).CAT24-Y(3);
                GO TO N12;
               END D37;
                YZX(2)=YZX(2)+OX(4).CAT24;
                IF YZX(2)<0.01 THEN GO TO N12;
                IF YZX(2)<0.10 THEN
                D40:DO;
                YZX(1)=YZX(1)+YZX(2);
                YZX(0)=YZX(0)+OX(4).CAT24;
```

```
                YZX(2)=-1;
                GO TO N12;
               END D40;
                YZX(0)=YZX(0)+CX(4).CAT24;
/* AL */  N12:IF YZX(1)<0.01 THEN GO TO N13;
                IF YZX(1)<0.10 & YZX(2)>0.10 THEN
           D41:DO;
                YZX(2)=YZX(2)+YZX(1);
                YZX(1)=-1;
                GO TO N13;
               END D41;
/* LI */  N13:IF OX(13).CAT24<0.01 THEN GO TO N14;
                Y(8)=OX(13).CAT24;
                Y(0)=Y(0)+Y(8);
/* NI,CO,ZN,MN */
           N14:N=11;
          N141:IF CX(N).CAT24<0.01 THEN
           D45:DO;
                N=N-1;
                IF N>7 THEN GO TO N141; ELSE GO TO N15;
               END D45;
                IF OX(N).CAT24¬>0.10 THEN
           D46:DO;
                Y(2)=Y(2)+OX(N).CAT24;
                Y(0)=Y(0)+CX(N).CAT24;
                Y(N-4)=-1;
                GO TO D45;
               END D46;
                Y(N-4)=OX(N).CAT24;
                Y(0)=Y(0)+Y(N-4);
                GO TO D45;
/*CU*/N15:IF OX(27).CAT24 < 0.01 THEN GOTO G3;
           IF OX(27).CAT24 ¬> 0.10 THEN
 D5000: DO;
           Y(2) = Y(2) + OX(27).CAT24;
```

```
          Y(0) = Y(0) + OX(27).CAT24;
        Y(13) = -1;
     END D5000;
          ELSE
 D4001:  DO;
        Y(13) = Y(13) + OX(27).CAT24;
        Y(0) = Y(0) +Y(13);
         END D4001;
/*,FEOUS */ G3: Y(2)=Y(2)+OX(7).CAT24;
              IF Y(2)<0.01 THEN GO TO N16;
              IF Y(2)¬>0.10 THEN
           D47:DO;
              Y(1)=Y(1)+Y(2);
              Y(0)=Y(0)+OX(7).CAT24: Y(2)=-1;
              GO TO N16;
             END D47;
              Y(0)=Y(0)+OX(7).CAT24;
/* MG */  N16:Y(1)=Y(1)+CX(12).CAT24;
              IF Y(1)<0.01 THEN GO TO N17;
              IF Y(1)¬>0.10 & Y(2)>0.10 THEN
           D48:DO;
              Y(2)=Y(2)+Y(1);
              Y(0)=Y(0)+OX(12).CAT24;
              Y(1)=-1;
              GO TO N17;
             END D48;
              Y(0)=Y(0)+OX(12).CAT24;
           N17:/*CHECK TOTALS*/
           D49:DO N=1 BY 1 TO 4;
              IF OH(N)>0 THEN
              Y(11)=Y(11)+OH(N);
             END D49;
IF ABS(Y(11)-OH(0))> 0.005 THEN RR(4)=1;
              Y(11)=C;
           D50:DO N=1 BY 1 TO 3;
```

```
                IF Z(N)>0  THEN
                Y(11)=Y(11)+Z(N);
               END D50;
IF ABS(Y(11)-Z(0))>0.005 THEN RR(5)=1;
                Y(11)=0;
           D51:DO N=1 TO 6;
                IF YZX(N)>0 THEN
                Y(11)=Y(11)+YZX(N);
               END D51;
IF ABS(Y(11)-YZX(0))> 0.005 THEN RR(6)=1;
           D52:DO N=1 BY 1 TO 10; IF Y(N)>0 THEN Y(11)=Y(11)+Y(N);
END D52; IF ABS(Y(11)-Y(0)-YZX(0))> 0.005 THEN RR(7)=1;
                Y(11)=0;
/* TI */        YZX(6)=YZX(6)+DX(15).CAT24;
                YZX(0)=YZX(0)+DX(15).CAT24;
                Y(12)=YZX(0)+Y(0);
                IF Y(12)>7.07 THEN J=1; ELSE
                IF Y(12)<=7.07 & Y(12)>6.90 THEN J=2; ELSE
                IF Y(12)<=6.90 & Y(12)>=6.50 THEN J=3;ELSE
                IF Y(12)<6.50  & Y(12)>=5.20 THEN J=4;ELSE
                IF Y(12)<5.20  & Y(12)>5.05 THEN J=5; ELSE
                J=6;
           IF J<6 THEN
D53:       DO;
           Y(12) = Y(12) - 5.00;
/* LI */   IF Y(8) -> 0.10 THEN GOTO G6;
           IF Y(8) >= Y(12) THEN
D54:      DO;
           X(6) = X(6) + Y(12);
           X(0) = X(0) + X(6);
           Y(8) = Y(8) - Y(12);
           Y(0) = Y(0) - Y(12);
           Y(12) = 0;
IF YZX(1)+YZX(2) <Y(8) THEN GOTO N18;
IF YZX(1)>Y(8) THEN DO;
```

```
Y(9)=Y(8);
Y(0)=Y(0)+Y(9);
YZX(1)=YZX(1)-Y(9);
YZX(0)=YZX(0)-Y(9);
GOTO N18; END;
IF YZX(2)> Y(8) THEN DO;
Y(10)=Y(8);
Y(0)=Y(0)+Y(10);
YZX(2)=YZX(2)-Y(10);
YZX(0)=YZX(0)-Y(10);
GOTO N18; END;
IF YZX(1)>YZX(2) THEN DO;
Y(9)=YZX(1); YZX(1)=0; YZX(0)=YZX(0)-Y(9);
Y(10)=Y(8)-Y(9); YZX(2)=YZX(2)-Y(10);
Y(0)=Y(0)+Y(9)+Y(10);
YZX(0)=YZX(0)-Y(10); GOTO N18;
END;
Y(10)=YZX(2); YZX(2)=0;
YZX(0)=YZX(0)-Y(10);
Y(9)=Y(8)-Y(10); YZX(1)=YZX(1)-Y(9);
Y(0)=Y(0)+Y(9)+Y(10);
YZX(0)=YZX(0)-Y(9);
          GOTO N18;
          END D54;
          X(6) = X(6) + Y(8);
       Y(0) = Y(0) - Y(8);
          Y(8) = 0;
          Y(12) = Y(12) - X(6);
    X(0) = X(0) + X(6);
G6:       IF Y(4) ¬> 0.10 THEN GOTO G7;
/*MN */  IF Y(4) >= Y(12) THEN
D4005:    DO;
          X(4) = X(4) + Y(12);
          X(0) = X(0) + X(4);
          Y(4) = Y(4) - Y(12);
```

```
          Y(0) = Y(0) - Y(12);
          Y(12) = 0;
         GOTO N18;
          END D4005;
          X(4) = X(4) + Y(4);
         X(0) = X(0) + X(4);
          Y(0) = Y(0) - Y(4);
          Y(4) = 0;
          Y(12) = Y(12) - X(4);
G7: IF Y(2)¬> 0.01 THEN GOTO G9;
 /*FEUS*/ IF Y(2) > Y(12) THEN
D4007:    DO;
          X(5) = X(5) + Y(12);
          X(0) = X(0) + X(5);
          Y(2) = Y(2) - Y(12);
          Y(0) = Y(0) - Y(12);
          Y(12) = 0;
          GOTO N18;
          END D4007;
          X(5) = X(5) + Y(2);
          X(0) = X(0) + X(5);
          Y(0) = Y(0) - Y(2);
          Y(2) = 0;
          Y(12) = Y(12) - X(5);
G9: /* CO */ IF Y(6)¬> 0.01 THEN GOTO G90;
          IF Y(6) > Y(12) THEN
D4006:    DO;
          X(9) = X(9)+ Y(12);
       X(0) = X(0) + X(9);
          Y(6) = Y(6) - Y(12);
          Y(0) = Y(0) - Y(12);
          Y(12) = 0;
          GOTO N18;
          END D4006;
          X(9) = X(9) + Y(6);
```

```
          X(0) = X(0) + X(9);
          Y(0) = Y(0) - X(9);
          Y(6) = 0;
          Y(12) = Y(12) - X(9);
G90: /* ZN */ IF Y(5)¬> 0.01 THEN GOTO G91;
IF Y(5)> Y(12) THEN DO;
X(10)=X(10)+Y(12);
X(0)=X(0)+X(10);
Y(5)=Y(5)-Y(12);
Y(0)=Y(0)-Y(12);
Y(12)=0.0;
GOTO N18; END;
X(10)=X(10)+Y(5);
X(0)=X(0)+X(10);
Y(0)=Y(0)-Y(5);
Y(5)=0.0;
Y(12)=Y(12)-X(10);
G91: /* CU */ IF Y(13)¬> 0.01 THEN GOTO G92;
IF Y(13) >Y(12) THEN DO;
X(11)=X(11)+Y(12);
X(0)=X(0)+X(11);
Y(13)=Y(13)-Y(12);
Y(0)=Y(0)-Y(12);
Y(12)=0.0;
GOTO N18; END;
X(11)=X(11)+Y(13);
X(0)=X(0)+X(11);
Y(0)=Y(0)-Y(13);
Y(13)=0.0;
Y(12)=Y(12)-X(11);
G92: /* MG */ IF Y(1)¬> 0.01 THEN GOTO G10;
          IF Y(1) > Y(12) THEN
D4008:    DO;
          X(3) = X(3) + Y(12);
        X(0) = X(0) + X(3);
```

```
          Y(1) = Y(1) - Y(12);
          Y(0) = Y(0) - Y(12);
          Y(12) = 0;
          GOTO N18;
          END D4008;
          X(3) = X(3) + Y(1);
          X(0) = X(0) + X(3);
          Y(0) = Y(0) - Y(1);
          Y(1) = 0;
        Y(12) = Y(12) - X(3);
IF Y(12)> 0.10 THEN RR(8)=1;
 Y(12) = 0;
  GOTO N18;
G10:      END D53;
IF Y(8)¬>0.01 THEN GOTO N100;
/* WITHIN Y SITE LI BALANCED AS LIAL OR LIFEIC */
IF YZX(1)+YZX(2)<Y(8) THEN GOTO G101;
                IF YZX(1)>Y(8) THEN
           D42:DO;
                Y(9)=Y(8);
                Y(0)=Y(0)+Y(9);
                YZX(1)=YZX(1)-Y(9);
                YZX(0)=YZX(0)-Y(9);
   GOTO N100;
               END D42;
                IF YZX(2)>Y(8) THEN
           D43:DO;
                Y(10)=Y(8);
                Y(0)=Y(0)+Y(10);
                YZX(2)=YZX(2)-Y(10);
                YZX(0)=YZX(0)-Y(10);
   GOTO N100;
               END D43;
                IF YZX(1)>YZX(2) THEN
           D44:DO;
```

```
                Y(9)=YZX(1); YZX(1)=0; YZX(0)=YZX(0)-Y(9);
                Y(10)=Y(8)-Y(9); YZX(2)=YZX(2)-Y(10);
                Y(0)=Y(0)+Y(9)+Y(10);
     YZX(0)=YZX(0)-Y(10); GOTO N100;
              END D44;
                Y(10)=YZX(2);  YZX(2)=0;
                YZX(0)=YZX(0)-Y(10);
                Y(9)=Y(8)-Y(10); YZX(1)=YZX(1)-Y(9);
                Y(0)=Y(0)+Y(9)+Y(10);
                YZX(0)=YZX(0)-Y(9);
GOTO N100;
G101:  RR(9)=1;
N100:           IF ROUND(Y(12),2)>=5.00 THEN
          D571:DO;
                Y(12)=0;
                GO TO N18;
               END D571;
/* Y SITE VACANCIES */
      Y(12) = 5.00 - Y(12);
/*TI VAC */    IF Y(12)<=YZX(6) THEN
           D58:DO;
                Y(11)=Y(12);
                Y(0)=Y(0)+2*Y(11);
                YZX(6)=YZX(6)-Y(11);
                YZX(0)=YZX(0)-Y(11);
                Y(12)=0;
                GO TO N18;
               END D58;
/*FEIC VAC */ IF Y(12)<=YZX(6)+YZX(2)/2 THEN
           D59:DO;
                Y(11)=YZX(6);
                YZX(0)=YZX(0)-YZX(6);
                YZX(6)=0;
                Y(0)=Y(0)+2*Y(11);
                Y(12)=Y(12)-Y(11);
```

```
Y(0)=Y(0)+3.0*Y(12);
YZX(0)=YZX(0)-2.0*Y(12);
YZX(2)=YZX(2)-2.0*Y(12);
Y(12)=2.0*Y(12);
                GO TO N18;
               END D59;
RR(10)=1;
                Y(12)=0;
/*X GRP*/ N18:IF OX(17).CAT24+OX(18).CAT24>0.10 THEN
RR(11)=1;
                IF X(0)>=2.00 THEN
            D60:DO;
                A(4)=OX(16).CAT24+OX(17).CAT24+OX(18).CAT24;
                A(1)=OX(19).CAT24;
                A(2)=OX(20).CAT24;
          A(6) =  OX(29).CAT24;
          DELTA = X(0) - 2.00;
   /* PROTOAMPHIBOLE LI TO A */
          IF X(6) ¬> DELTA THEN GOTO G11;
           A(5) = A(5) + DELTA;
           X(6) = X(6) - DELTA;
           X(0) = X(0) - DELTA;
         A(0) =A(0) +A(1)+A(2)+A(4)+A(5)+A(6);
          GOTO N19;
G11:      A(0) = A(0) +A(1)+A(2)+A(4)+A(6);
                GO TO N19;
               END D60;
           X(2) = 2.00 - X(0);
           X(1) = OX(16).CAT24+OX(17).CAT24+OX(18).CAT24;
           X(7) = OX(29).CAT24;
           X(8) = OX(28).CAT24;
/*CD*/     IF ROUND(X(8),2) >= X(2) THEN
D4010:     DO;
           A(7) = X(8) - X(2);
           X(8) = X(2);
```

```
            X(0) = X(0) + X(8);
            X(2) = 0;
            A(6) = X(7);
            A(1) = OX(19).CAT24;
            A(2) = OX(20).CAT24;
            A(4) = X(1);
            X(1) = 0; X(7) = 0;
          A(0) = A(0)+A(1)+A(2)+A(4)+A(6)+A(7);
            GOTO N19;
            END D4010;
            X(0) = X(0) + X(8);
/*CA BA SR */ X(2) = 2.00 - X(0);
            IF ROUND (X(1),2) >= X(2) THEN
D4011:      DO;
            A(4) = X(1) - X(2);
            X(1) = X(2);
            X(0) = X(0) + X(1);
            A(1) = OX(19).CAT24;
            A(2) = OX(20).CAT24;
            A(6) = X(7);
            X(2) = 0;
            A(0) = A(0) + A(1)+A(2)+A(6)+A(4);
            X(7) = 0;
            GOTO N19;
            END D4011;
/*PB*/      X(2) = 2.00 - X(0);
            IF RCUND(X(7),2) >= X(2)THEN
D4012:      DO;
            A(6) = X(7)- X(2);
            X(7) = X(2);
            X(2) = 0;
            X(0) = X(0) + X(7);
            A(1) = OX(19).CAT24;
            A(2) = OX(20).CAT24;
            A(0) = A(0) + A(6) + A(1) + A(2);
```

```
          GOTC N19;
         END D4012;
         X(0) = X(0)+ X(7);
          X(2) = 2.00 - X(0);
          IF X(1) + OX(19).CAT24 >=X(2) THEN
           D62:DO;
               X(2)=X(2)-X(1);
               X(0)=X(0)+X(1)+X(2);
               AX(1)=OX(19).CAT24-X(2);
               IF AX(1)>=X(2) THEN
           D63:DO;
               A(1)=AX(1)-X(2);
               AX(1)=X(2);
               A(2)=OX(20).CAT24;
               A(0)=A(0)+A(1)+A(2);
               AX(0)=AX(0)+AX(1);
               GO TO N19;
              END D63;
               IF AX(1)+OX(20).CAT24>=X(2) THEN
           D64:DO;
               A(2)=OX(20).CAT24-X(2)+AX(1);
               AX(2)=OX(20).CAT24-A(2);
               A(0)=A(0)+A(2);
               AX(0)=AX(0)+AX(1)+AX(2);
               GO TO N19;
              END D64;
               AX(2)=OX(20).CAT24;
               AX(0)=AX(0)+AX(1)+AX(2);
               GO TO N19;
              END D62;
RR(12)=1;
               X(2)=OX(19).CAT24;
               X(0)=X(0)+X(1)+X(2);
               A(2)=OX(20).CAT24;
               A(0)=A(0)+A(2);
```

```
N19: RETURN;
END AXYZ;
```

APPENDIX 5.

DATA BASE PROGRAMS LOAD AND QUERY.

The computer programs written by the author in PL/1 to act as a versatile data base for the amphibole data file are described below.

A5.1. LOAD: Program Function.

Program LOAD is used to load data, which has a hierarchical or tree organisation, sequentially, onto a file. In order to make the program independent of the specific hierarchical organisation in use at any time the organisation is input as data rather than defined within the program. The organisation is defined by inputing for each elementary level and node in a n-level tree, n-1 level numbers, the name of the elementary level or node and the mode of the possible response if any, see Chapter 4 for details. Where alternative names for nodes or elementary levels are required these also can be input. Once the organisation has been input data follows. Data input is similar to PL/1 'data directed' input, with each item of data (response) consisting of three parts (i) the reference number of the object to which the response refers, (ii) the name of the elementary level to which data is to be directed and (iii) the response itself. The elementary level name is matched with the possible elementary level names or their alternatives and replaced by an integer compounded from the appropriate n-1 level numbers. Each response is then entered sequentially onto a line file as four items, (i) the number of the object, (ii) the compounded level number, (iii) the mode and (iv) the response.

Data Input.

Three integers, NL the number of levels in the tree, NE the total number of elementary levels and nodes in the tree and NQ the total number of alternative names for elementary levels and nodes are input initially. Data input is list directed, that is, each number is

separated from the following by an intervening blank or comma. When there are no alternative names, NQ must still be input as 0.

Characteristics of the hierarchical organisation are input next. For each of the NE elementary levels and nodes, the n-1 level numbers, their names and data modes are read, in the above order, from a line file C. Input is list directed. The level numbers and the mode are integers, the name is a character string with a maximum length of 25 characters. The name must be enclosed in quotation marks but may consist of any combination of alphanumeric characters with the restriction that an internal quotation mark must be double. Modes for responses are coded as follows, 0 for a node, 1 character string, 2 integar, 3 floating point number. Thus in a four level tree the following is a valid entry for an elementary level:- 2,3,0, 'HOSTROCK', 1, .

Where there are alternative names for elementary levels, then for each of the NQ alternatives the following is input, n-1 level numbers, and the alternative name. Input is again list directed and subject to the same restrictions as above. If HOST is an abbreviated alternative for HOSTROCK then this would be input as :- 2,3,0 'HOST', .

Lastly the data to be stored is input. For each response an integar identifier of the corresponding object, the name of the elementary level (property) the response refers to and the response itself are input. Input is list directed, e.g. 1, 'HOST', 'AMPHIBOLITE', 1,'SIO2', 56.74, etc. The name must be that of an elementary level or its alternatives. There is no need to mark the end of the data.

Implementation.

LOAD, written in PL/1, requires two files. File C is

used to store the data organisation and file STORE is used to store the data. Both are required by the QUERY program see A5.2.

Table A5.1. Listing of program LOAD.

```
LOAD: PROC OPTIONS(MAIN);

/*   PL/1   */

/*   J.L. KNIGHT  1972  */

/*   DATA LOADING PROGRAM   */

/*   REQUIRES TWO LINE FILES, C AND STORE  */

GET LIST(NL,NE,NG);
BEGIN;
DCL (A(NE,NL),TYPE(NE),EGA(NG,NL),B(NL),N(NL),VINT,TYP) FIXED BIN;
DCL (NAME(NE),EGNAM(NG),NAM) CHAR(25);
DCL VCHAR CHAR(80);
DCL TNC FIXED BIN;
DCL (C) FILE;
DCL (STORE) FILE;
ON ENDFILE(SYSIN) GOTO FIN;
DCL LAB(7) LABEL INIT(L1,L2,L3,L4,L5,L6);
N=NL-1;
A=0; TYPE=0; NAME=' ';

/* READ IN THE LEVEL NUMBERS, NAMES AND MODES OF THE ELEMENTARY LEVELS AND
NODES IN THE HIERARCHICAL STRUCTURE */

DO I = 1 TO NE;
GET FILE(C) LIST((A(I,J) DO J = 1 TO NL),NAME(I),TYPE(I));
PUT EDIT((A(I,J) DO J = 1 TO NL),TYPE(I),NAME(I))(3 F(5),A);
END;
IF NG=0 THEN GOTO S2F;

/* READ IN THE LEVEL NUMBERS AND ALTERNATIVE NAMES FOR ELEMENTARY LEVELS OR
NODES IN THE HIERARCHICAL STRUCTURE */
```

```
DO I = 1 TO NQ;
GET FILE(C) LIST((EQA(I,J) DO J = 1 TO NL),EQNAM(I));
PUT EDIT((EQA(I,J) DO J = 1 TO NL),EQNAM(I))(3 F(5),A); END;
S20: CLOSE FILE(C);
OPEN FILE(STORE) OUTPUT;
G1:          N=0;II=0;VFL=0;VINT=0;NAM=' ';VCHAR=' ';
TNO=0;

/* READ IN DATA */

GET LIST(TNO,NAM);
PUT LIST(TNO,NAM);

/* MATCH THE ELEMENTARY LEVEL NAME IN THE DATA WITH ELEMENTARY LEVEL NAMES
IN THE HIERARCHICAL STRUCTURE AND DETERMINE THE APPROPRIATE LEVEL NUMBERS */

DO I = 1 TO NE;
IF NAM=NAME(I) THEN DO;
II=TYPE(I);
DO K = 1 TO NL;
N(K)=A(I,K);
END;
GOTO G2; END;
END;

/* IF NO MATCH WAS ACHIEVED TRY MATCHING THE ELEMENTARY LEVEL NAME IN THE
DATA WITH ALTERNATIVE NAMES FOR ELEMENTARY LEVELS IN THE HIERARCHICAL STRUCTURE
     */
IF N(1)=0 THEN DO;
DO I = 1 TO NQ;
IF NAM=EQNAM(I) THEN DO;
DO K = 1 TO NL;
N(K)=EQA(I,K);
END;
DO K = 1 TO NE;
```

```
KK=C;
DC L = 1 TC NL;
IF N(L)=A(K,L) THEN KK=KK+1; END;
IF KK=NL THEN DC;
II=TYPE(K); GCTC G2; END;
END; END;
END;
PUT EDIT('NAME CAN NCT BE ICENTIFIED',NAM)(COL(20),A,X(2),A);
GCTC FIN;
END;

/* HASH LEVEL NUMBERS */

G2:IHASH=0;
DC I = 1 TC NL;
M=2*I;
IHASH=IHASH+N(I)*10**M;
END;
PUT LIST(IHASH);
GCTC LAB(II);
L1: GET LIST(VCHAR); GCTC L4;
L2: GET LIST(VINT); GOTO L5;
L3: GET LIST(VFL); GCTC L6;

/* LCAC CATA CNTC FILE STCRE */

L4:PUT FILE(STCRE) EDIT(TNO,IHASH,II)
(X(1),F(5),X(1),F(20),X(1),F(2));
PUT FILE(STCRE) EDIT(VCHAR)(X(1),A(80));
PUT EDIT(TNO,IHASH,II,VCHAR)
(X(1),F(5),X(1),F(20),X(1),F(2),X(1),A);        GOTO FL;
L5:PUT FILE(STCRE) EDIT(TNC,IHASH,II)
(X(1),F(5),X(1),F(2C),X(1),F(2));
PUT FILE(STCRE) EDIT(VINT)(X(1),F(5));
PUT EDIT(TNC,IHASH,II,VINT)
```

```
(X(1),F(5),X(1),F(20),X(1),F(2),X(1),F(5));          GOTO G1;
L6: PUT FILE(STORE) EDIT(TNC,IHASH,II)
(X(1),F(5),X(1),F(20),X(1),F(2));
PUT FILE (STORE) EDIT(VFL) (X(1),F(9,3));
PUT EDIT(TNC,IHASH,II,VFL)
(X(1),F(5),X(1),F(20),X(1),F(2),X(1),F(8,3));          GOTO G1;
FIN: CLOSE FILE(STORE);
END; END;
```

A5.2. QUERY: Program Function.

Program QUERY is used to set a query of data loaded sequentially onto a line file by LOAD. The query itself, in the form of a modified PL/1 'IF statement' and the names of those elementary levels for which responses are required if the query is found to be 'true' are read in as data. In this way the program is independant of the particular query and data organisation.

Data Input.

For each query four integers are input initially. NL the number of levels in the hierarchical structure, M the number of separate logical comparisons in the query, NO the number of elementary levels for which data is required to be output, and MAX a value equal to, or greater than, the number of objects currently in the data file. Data input is list directed. This is followed by the query. For example if the data is organised as Table 4.1 a query for the literature source of those amphiboles named kaersutite or with TiO_2 greater than 10 weight per cent is given by : -

'NAME' '=' 1 'KAERSUTITE' 'OR' 'TIO2' '>' 3 10.0

'AUTHOR' 1 'AUTHORINITIALS' 1 'DATE' 2 'JOURNAL' 1

The first line as written above defines the logic of the query and is of the general form

'PROPERTY' 'COMPARISON' DATA MODE 'CRITICAL RESPONSE' 'LOGICAL OPERATOR'

'PROPERTY' 'COMPARISON' DATA MODE 'CRITICAL RESPONSE' (- - - etc)

where

PROPERTY is the name of any elementary level in the hierarchical structure,

COMPARISON is one of the following

'=' equal to '¬=' not equal to

'>' greater than '¬>' not greater than

'<' less than '¬<' not less than

DATA MODE is the mode of the property

1 character string 2 integer

3 floating point number,

CRITICAL RESPONSE is the critical value of the response to be tested,

LOGICAL OPERATOR either 'AND' or 'OR'.

In interpreting the logic of the query the program works from left to right. No parantheses are allowed.

The second part of the query consists of a list of the names and data modes of elementary levels for which data is to be output if the query is 'true'. These are input in the general form

'PROPERTY' DATA MODE

Implementation

QUERY, written in PL/1, requires two line files C and STORE (see LOAD), and an external subroutine TRANS.

Table A5.2. Listing of program QUERY.

```
QUERY: PROC OPTIONS(MAIN);

/*    PL/1    */
/*    QUERY PROGRAM    */

/*    REQUIRES THE EXTERNAL SUBROUTINE TRANS AND TWO LINE FILES C AND STORE*/

/*     QUERY IS A PROGRAM TO SET A QUERY OF DATA LOADED SEQUENTIALLY ONTO A LINE
       FILE BY PROGRAM LOAD. THE QUERY ITSELF IS INPUT IN THE FORM OF A
       MODIFIED PL/1 'IF STATEMENT'.          */

ON ENDFILE(SCARDS) GOTO FINI;
AGAIN: GET LIST(NL,M,NO,MAX);
BEGIN;
DCL NAME(M) CHAR(20),COMP(M) CHAR(2),TYPE(M) FIXED BIN;
DCL VCHAR(M) CHAR(80),VINT(M) FIXED BIN,VFL(M)  FLOAT,LOG(M) CHAR(3);
DCL LAB(3) LABEL INIT(L1,L2,L3);
DCL OUTPUT(NO) CHAR(20);
DCL (TTYPE(3,M),IT(3),REPLY,SKIP(M)) FIXED BIN;
DCL ( HASH(M),VVINT)FIXED BIN;
DCL VVCHAR CHAR(80);
DCL SKIP2(M) FIXED BIN;
DCL (TRYPE(NO),THASH(NO),IR(3),TTT(3,NO)) FIXED BIN;
DCL TRANS ENTRY(CHAR(20),FIXED BIN,FIXED BIN);
DCL STORE FILE;

NAME,OUTPUT=' ';
COMP=' ';
TRYPE=0;
IT=0;
IR=0;
TTT=0;
TYPE,VINT,SKIP,HASH=0;
VCHAR=' '; VFL=0;
LOG=' ';
```

```
TTYPE=0;VVINT=0;VVCHAR=' ';
IT=0;
NL=NL-1;

/* READ IN QUERY */

DO I = 1 TO M;
GET LIST(NAME(I),COMP(I),TYPE(I));
GOTO LAB(TYPE(I));
L1: GET LIST(VCHAR(I));
PUT EDIT(VCHAR(I)) (X(1),A); GOTO G1;
L2: GET LIST(VINT(I));
PUT EDIT(VINT(I))(X(1),F(5)); GOTO G1;
L3: GET LIST(VFL(I));
PUT EDIT(VFL(I))(X(1),F(10,5)); GOTO G1;
G1: IF I<=M-1 THEN DO;
GET LIST(LOG(I));
END; END;

/* READ IN ELEMENTARY LEVELS TO BE OUTPUT */

PUT EDIT('OUTPUT FIELDS ARE AS FOLLOWS')(COL(20),A);

DO I=1 TO NO;
GET LIST(OUTPUT(I),TRYPE(I));
PUT EDIT(OUTPUT(I))(X(5),A);
END;

G5: DO I = 1 TO M;
IF TYPE(I)=1 THEN DO;
 IT(I)=IT(I)+1;TTYPE(1,I)=IT(1); GOTO G2; END;
IF TYPE(I)=2 THEN DO;
IT(2)=IT(2)+1; TTYPE(2,I)=IT(2); GOTO G2; END;
IF TYPE(I)=3 THEN DO;
IT(3)=IT(3)+1; TTYPE(3,I)=IT(3); END;
```

```
G2: END;

DO I = 1 TO NO;
IF TRYPE(I)=1 THEN DO;
IR(1)=IR(1)+1; TTT(1,I)=IR(1); GOTO G10; END;
IF TRYPE(I)=2 THEN DO;
IR(2)=IR(2)+1; TTT(2,I)=IR(2); GOTO G10; END;
IF TRYPE(I)=3 THEN DO;
IR(3)=IR(3)+1; TTT(3,I)=IR(3); GOTO G10; END;
G10; END;

/* SET UP LOGICAL FLOW*/

DO I = 1 TO M;
SKIP(I)=I+1;
END;

SKIP2=0;
SKIP2(M)=M+1;

DO I = 1 TO M-1;
IF LOG(I)='OR' THEN SKIP2(I)=I+1;
END;

DO I = M TO 1 BY -1;
IF SKIP2(I)=0 THEN SKIP2(I)=SKIP2(I+1); END;
DO I = 1 TO M;

IF M=1 THEN DO; SKIP=2; GOTO G3; END;

DO I = 1 TO M-1;
IF LOG(I)='AND' THEN SKIP(I)=I+1;
IF LOG(I)='OR' THEN SKIP(I)=M+1;
END;
```

```
G3: /*TRANSLATE NAMES INTO HASHED FORM*/

HASH=0;
DO I = 1 TO M;
CALL TRANS(NAME(I),HASH(I),NL);
END;
THASH=0;
DO I = 1 TO NO;
CALL TRANS(OUTPUT(I),THASH(I),NL);
END;

/* READ IN DATA AND SET QUERY */

M1=IT(1)+1; M2=IT(2)+1;M3=IT(3)+1;
M4=IR(1)+1; M5=IR(2)+1; M6=IR(3)+1;
BEGIN;
DCL PATH(M+1) LABEL;
DCL (CHAR(MAX,M1),OCHAR(MAX,M4)) CHAR(80);
DCL (INT(MAX,M2),OINT(MAX,M5))FIXED BIN;
DCL (FL(MAX,M3),OFL(MAX,M6)) FLOAT;
DCL LAC(3) LABEL INIT(L4,L5,L6);
DCL RESULT(MAX) BIT(1);
ON ENDFILE(STORE) GOTO G8;
OINT=-2234; INT=-1234;
OFL = 1234.567; FL=1234.567;
CHAR='AAXXCCVV'; OCHAR='AAXXCCVV';

DO I = 1 TO M+1;
PATH(I)=COMPLETE;
END;
DO I = 1 TO M;
IF COMP(I)='=' THEN PATH(I)=EQ;
IF COMP(I)='>' THEN PATH(I)=GT;
IF COMP(I)='<' THEN PATH(I)=LT;
IF COMP(I)='>='|COMP(I)=']<' THEN PATH(I)=GE;
```

```
IF COMP(I)='<='↑COMP(I)='>' THEN PATH(I)=LE;
IF COMP(I)='=' THEN PATH(I)=NEQ;
END;
OPEN FILE(STORE) INPUT;

DO I = 1 TO MAX;
GET FILE(STORE) EDIT(ISPEC,IHASH,ITYPE)
(X(1),F(5),X(1),F(20),X(1),F(2));
GOTO LAC(ITYPE);
L4: GET FILE(STORE) EDIT(VVCHAR) (X(1),A(80)); GOTO G4;
L5: GET FILE(STORE) EDIT(VVINT)(X(1),F(5)); GOTO G4;
L6: GET FILE(STORE) EDIT(VVFL)(X(1),F(8,3)); GOTO G4;
G4: DO I = 1 TO M;
IF IHASH=HASH(I) THEN DO;
IF TYPE(I)=1 THEN CHAR(ISPEC,TTYPE(1,I))=VVCHAR;
IF TYPE(I)=2 THEN INT(ISPEC,TTYPE(2,I))=VVINT;
IF TYPE(I)=3 THEN FL(ISPEC,TTYPE(3,I))=VVFL;
END; END;
DO I = 1 TO NO;
IF THASH(I)=IHASH THEN DO;
IF TRYPE(I)=1 THEN OCHAR(ISPEC,TTT(1,I))=VVCHAR;
IF TRYPE(I)=2 THEN OINT(ISPEC,TTT(2,I))=VVINT;
IF TRYPE(I)=3 THEN OFL(ISPEC,TTT(3,I))=VVFL;
END; END; END;

G8: CLOSE FILE(STORE);

/* SET QUERY*/

RESULT='0'B;
DO J = 1 TO MAX;

/* APPLY LOGICAL TEST TO DATA */

I=0;
```

```
DO L=1 TO M;
I=I+1;
IF I>M+1 THEN GOTO COMPLETE;
IF I=1 THEN  GOTO PATH(1);
IF RESULT(J) THEN GOTO PATH(SKIP(I-1));
IF LOG(I-1)='AND' THEN DO;
I=SKIP2(I-1); GOTO PATH(SKIP2(I-1)); END;
GOTO PATH(I);

EQ:
DO; IF TYPE(I)=1 THEN DO;
IF CHAR(J,TTYPE(1,I)) =VCHAR(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,1)) =VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I))=VFL(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;

GT:
DO; IF TYPE(I)=1 THEN DO;
PUT LIST('INAPPROPRIATE QUERY'); GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,I)) >VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I))>VFL(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;
```

```
PUT LIST('LT');
DO; IF TYPE(I)=1 THEN DO;
PUT LIST('INAPPROPRIATE QUERY'); GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,I)) <VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I))<VFL(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;

GE:
DO; IF TYPE(I)=1 THEN DO;
PUT LIST('INAPPROPRIATE QUERY'); GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,I))>=VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I)) >=VFL(I) THEN RESULT='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;

LE:
DO; IF TYPE(I)=1 THEN DO;
PUT LIST('INAPPROPRIATE QUERY'); GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,I))<=VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I)) <=VFL(I) THEN RESULT='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;
```

```
NEQ:
DO; IF TYPE(I)=1 THEN DO;
IF CHAR(J,TTYPE(1,I))]=VCHAR(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=2 THEN DO;
IF INT(J,TTYPE(2,I))]=VINT(I) THEN RESULT(J)='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END;
IF TYPE(I)=3 THEN DO;
IF FL(J,TTYPE(3,I)) ]=VFL(I) THEN RESULT='1'B;
ELSE RESULT(J)='0'B;
GOTO G6; END; END;


G6; END;

COMPLETE; END;

/* PRINT OUT RESULTS*/

DO J = 1 TO MAX;
IF RESULT(J) THEN DO;
PUT EDIT(J)(X(2),F(5));
DO K = 1 TO NO;
IF TRYPE(K)=1 THEN PUT LIST(OCHAR(J,TTT(1,K)));
IF TRYPE(K)=2 THEN PUT LIST(OINT(J,TTT(2,K)));
IF TRYPE(K)=3 THEN PUT LIST(OFL(J,TTT(3,K)));
END; END; END;
END;
END;

PUT LIST('NEXT QUERY');
GOTO AGAIN;
```

```
FINI: END;
```

Table A5.3. Listing of subroutine TRANS.

```
TRANS: PROC(NN,IH,N);

/*   PL/1   */

/* J.L. KNIGHT  1972  */

/*   SUBROUTINE TRANS  */

/* REQUIRES LINE FILE C */

DCL C FILE, A(N) FIXED BIN;
DCL (NN,NNN) CHAR(20);
ON ENDFILE(C) GOTO G1;
IH=0;
DO I = 1 TO 1000;
GET FILE(C) LIST((A(J) DO J = 1 TO N),NNN,IT);
IF NNN=NN THEN DO;
DO J = 1 TO N;
M=2*J;
IH=IH+A(J)*10**M;
END; GOTO G1; END;
END;
G1: RETURN; END;
```

APPENDIX 6.

SET OPERATIONS.

Manipulation of data in the form of relations may be undertaken by the set operations union, intersection, difference, selection, join and projection. The result of applying each of these operations to a relation, or relations, is a further relation. A simple explanation of the operations is given below along with examples (Table A6.1) involving relations containing imaginary information about the authors of a number of scientific articles. For a more detailed discussion see Codd (1970) and Notley (1972).

union - Forms an unpurged union of two relations both of the same degree. The cardinality of the resultant relation is the sum of that of the two relations. Duplication of tuples is not removed, e.g. the union of SENIOR-AUTHOR and OTHER-AUTHORS yields AUTHORS.

Intersection - Forms a new relation of all the tuples common to two relations both of the same degree, e.g. the intersection of SENIOR-AUTHOR with AUTHORS is SENIOR-AUTHOR.

Difference - Forms a new relation of all the tuples of one relation which are not common to two relations both of the same degree, e.g. the difference of SENIOR-AUTHOR with AUTHORS is OTHER-AUTHORS.

Selection - Removes from a relation all those tuples for which some logical filter is false and leaves a relation of those tuples for which the filter is true, e.g. a selection of AUTHORS with the filter DATA = 1930 leaves YEAR.

Join - Concatenates the tuples of two relations (of the same or different degrees) about a common domain, e.g. the join between SENIOR-AUTHOR and OTHER-AUTHORS about domain REF # produces JOINT-AUTHORS.

Projection - Forms a new relation consisting of some of the domains of another relation. Duplicated tupes are eliminated, e.g. REFERENCE is one of the projections of JOINT-AUTHORS.

TABLE A6.1. Examples of set operations.

SENIOR-AUTHOR	(REF #,	NAME,	DATE)
	1	A	1930
	2	B	1960
	3	C	1970
	4	D	1952
OTHER-AUTHORS	(REF #,	NAME,	DATE)
	1	C	1930
	2	E	1960
AUTHORS	(REF #,	NAME,	DATE)
	1	A	1930
	2	B	1960
	3	C	1970
	4	D	1952
	1	C	1930
	2	E	1960
YEAR	(REF #,	NAME,	DATE)
	1	A	1930
	1	C	1930

JOINT AUTHORS	(REF # 1,	NAME 1,	DATE 1,	REF # 2,	NAME2,	DATE2)
	1	A	1930	1	C	1930
	2	B	1960	2	E	1960

REFERENCE	(NAME 1,	NAME 2,	DATE)
	A	C	1930
	B	E	1960

APPENDIX 7.

DATA CHARACTERISTICS OF RELATIONS IN THE AMPHIBOLE DATA BASE.

Data modes are abbreviated as follows:-

1 character string,

2 integer,

3 floating point number.

RELATION NAME	DOMAIN NAME	DOMAIN NO.	DATA MODE	LENGTH OF FIELD
REFERENCE	REF.NO.	1	2	6
	AUTHOR	2	1	19
	AUTHORINTIALS	3	1	6
	ANALYST	4	1	21
	ANALYSTINITIALS	5	1	6
	DATE	6	2	4
	REFERENCE	7	1	59
	VOLUME	8	1	34
ANALYSIS	REF.NO.	1	2	6
	REF.CODE.	2	1	14
MINERALNAME	REF.NO.	1	2	6
	NAME	2	1	74
GEOGRAPHY	REF.NO.	1	2	6
	COUNTRY	2	1	16
	COUNTY	3	1	18
	LOCALITY	4	1	20
OCCURRENCE	REF.NO.	1	2	6
	ROCKNAME	2	1	34
OPTICS	REF.NO.	1	2	6
	ALPHA	2	3	6
	ALPHAERROR	3	3	6
	BETA	4	3	6
	BETAERROR	5	3	6
	GAMMA	6	3	6
	GAMMAERROR	7	3	6
	2V	8	3	6
	DISPERSION	9	1	4
	ORIENTATION	10	1	18
	O.A.P.	11	1	10
	DELTA.	12	3	6
	DELTAERROR	13	3	6
	EXT.L.	14	1	18
COLOUR	REF.NO.	1	2	6
	COLOUR	2	1	74

PLEOCHROISM	REF.NO.	1	2	6
	FORMULA	2	1	5
	X	3	1	20
	Y	4	1	20
	Z	5	1	20
CHEMISTRY	REF.NO.	1	2	6
	OXIDE	2	1	8
	VALUE	3	3	
TRACE	REF.NO.	1	2	6
	ELEMENT	2	1	3
	VALUE	3	2	55
TECHNIQUE	REF.NO.	1	2	6
	EXAMINATION	2	1	2
	ANALYTICAL_METHOD	3	1	55
PHYSICAL	REF.NO.	1	2	6
	PROPERTY	2	1	8
	VALUE	3	3	6
STRUCTURE	REF.NO.	1	2	5
	CELLPARAMETER	2	1	7
	VALUE	3	3	7
	ERROR	4	3	7
SYMMETRY	REF.NO.	1	2	5
	SYMMETRY	2	1	14
COEXISTENCE	REF.NO.	1	2	6
	OTHER_REF.NO.	2	2	6
EXTRA	REF.NO.	1	2	6
	OTHER_REF.NO.	2	2	6
REDETERMINATION	REF.NO.	1	2	6
	OTHER_REF.NO.	2	2	6
ATOMIC_FORMULA	REF.NO.	1	2	6
	LARGEST_OXIDE	2	1	5
	LARGEST_VALUE	3	3	6
	SECOND_OXIDE	4	1	5

	SECOND_VALUE	5	3	6
	THIRD_VALUE	7	3	6
	24(0)SI	8	3	5
	24(0)P	9	3	5
	24(0)AL	10	3	5
	24(0)FEIC	11	3	5
	24(0)CR	12	3	5
	24(0)V	13	3	5
	24(0)FEDUS	14	3	5
	24(0)MN	15	3	5
	24(0)ZN	16	3	5
	24(0)CU	17	3	5
	24(0)NIO	18	3	5
	24(0)MG	19	3	5
	24(0)LI	20	3	5
	24(0)ZR	21	3	5
	24(0)TI	22	3	5
	24(0)CA	23	3	5
	24(0)BA	24	3	5
	24(0)SR	25	3	5
	24(0)NA	26	3	5
	24(0)K	27	3	5
	24(0)H	28	3	5
	24(0)OH	29	3	5
	24(0)F	30	3	5
	24(0)CL	31	3	5
	24(0)CO2	32	3	5
	24(0)S	33	3	5
	24(0)CU	34	3	5
	24(0)CO	35	3	5
	24(0)PB	36	3	5
	24(0)BE	37	3	5
	24(0)B	38	3	5
	23(0)SI	39	3	5
	- - - - - - AS ABOVE - - - - -			
	23(0)B	69	3	5
BASIC_FORMULA	REF.NO.	1	2	5
	24(0)NAA	2	3	5
	24(0)NAX	3	3	5
	24(0)ALY	4	3	5
	24(0)ALZ	5	3	5
	24(0)NAME	6	1	2

OH-2.0	7	3	6
24(O)CA_IN_A	8	3	5
24(O)MG_IN_X	9	3	5
23(O)NAA	10	3	5
23(O)NAX	11	3	5
23(O)ALY	12	3	5
23(O)ALZ	13	3	5
23(O)NAME	14	1	2
23(O)CA_IN_A	15	3	5
23(O)MG_IN_X	16	3	5

APPENDIX 8

SOURCE OF DATA IN THE AMPHIBOLE DATA FILE

A systematic search of the journals available in the Geology section of the University of Durham Science Library was made for articles published after 1900 containing a 'major element chemical analysis' of an amphibole. Reference to all such articles was kept on a card file. In addition to these, articles mentioned in Deer, Howie & Zussman (1963) and Leake (1968) or referred to in an article already in the card file were added. In all 1052 references were obtained. The card file is lodged with Mr. R. Phillips, Dept. Geological Sciences, Univ. Durham. Such a collection is by no means exhaustive and is biased towards English language journals.

Articles referred to in the card file were searched systematically for relevant information. Wherever possible the author's data was transcribed directly from the original source. Where this was not possible data was taken from a secondary source, in particular Leake (1968).

A complete list of the source of the analyses is given in Table A8.1 and in Table A8.2 the silica content and the name and value of the next largest oxide in each analysis is given. These can be used together to locate the original information for any specific amphibole in the data file.

In all 2205 entries taken from 654 primary sources have been included in the data file. In addition, 648 entries from secondary sources have also been included and represent about 23 per cent of the total of 2853 entries. These entries from secondary sources have in turn been obtained from 405 primary sources. The total of 2853 entries includes data for 2650 different amphiboles, the remaining 203 entries represent additional data published separately concerning one of the amphiboles in the data file.

It is probably true to say that this collection of data

represents only a small fraction of the total data available concerning amphiboles. Additional data is to be found in non-English language journals and unpublished sources. The addition of extra data to the data file is a simple but time consuming operation.

Table 4C.1. Literature source of chemical analyses in the amphibole data file.

Adams, F. D. (1903) In: Billings, M. (1928) Am. Miner., 13, 287-296, (183).

————, & Harrington, B. J. (1896) In: Leake, B. E. (1968) Geol. Soc. Amer. Spec. Paper., 98, 210pp, (10).

Addison, W. E., & Sharp, J. H. (1968) Mineral. Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting, Cambridge 1966), 305-311, (189).

Ahlfield, F. (1943) In: Drysdall, A. R., Newton, A. R. (1960) Am. Miner., 45, 55-59, (488-489).

Ainberg, L.F. (1930) In: Leake, B. E. (1968) op. cit., (11,533).

Alderman, A. R. (1936) Q. Jl. geol. soc. Lond., 92, 488-530, (2).

Allen, E. T., & Clement, J. K. (1908) Am. J. Sci., 26, 101-118, (5-9).

Allen, R. D., & Kramer, H. (1956) Am. Miner., 40, 527-530, (12).

Allen, V. T., Fahey, J. J. (1956) Bull. Geol. Soc. Amer., 67, 1664-1665, (13).

Alonsi, P. (1912) In: Leake, B. E. (1968) op. cit., (14).

Amin, M. S., & Afrifa, M. S. (1954) Econ. Geol., 49, 317-327, (15).

Andreatta, C., & Pirani, R. (1950) In: Leake, B. E. (1968), (16).

Angel, F., & Hartiny, G. (1925) Ibid.

Annersten, H., & Ekstrom, T (1971) Lithos, 4, 185-204, (18-32).

Aoki, K. (1959) In: Aoki, K. (1963) J. Petrology, 4, 198-210, (36).

————, (1961) In: Leake, B. E. (1968) op. cit. (33).

————, (1963) J. Petrology, 4, 198-210, (35,37,38,40,42-46).

————, (1964) Am. Miner., 49, 1199-1223, (47,49,51).

————, (1970) Contr. Mineral. and petrology, 25, 270-283, (55-61).

————, (1971) Ibid, 30, 314-331, (62-72).

————, & Kushiro, I (1964) Ibid, 18, 326-337, (73).

Appleyard, E. C. In: Leake, B. E. (1968) op. cit., (74-88).

Babkine, J., Bolfa, J., Roither, J. C., & Zoller, C. (1968) Mineral. Soc. I.M.A. (I.M.A. Papers and proc. 5th gen. meeting Cambridge 1966), 184-188, (74-88).

Bain, A. D. F. (1934) Q. Jl. Geol. Soc. Lond., 90, 201-236., (90).

Baker, C. (1959) In: Leake, B. E. (1968) op. cit., (89).

Bancroft, G. M., & Burns, R. G. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 137-148, (2501,2504,2512-2515).

Bancroft, J. A., & Howard, W. V. (1923) In: Leake, B. E. (1968) and Billings, M. (1928) Am. Miner., 13, 267-296, (92,104).

Banno, S. (1964) J. Fac. Sci. Tokyo Univ., 15, 203-319, (93-103, 105-110).

_____, et al. (1964) In: Leake, B. E. op. cit., (111, 534, 575).

Bard, J. P. (1970) Contr. Mineral. and Petrology, 28, 117-134, (112-131).

Barnes, V. E. (1930) Am. Miner., 15, 393-417, (132-135,2530-2535).

Barth, T. F. W. (1930) In: Leake, B. E. op. cit., (136,576).

_____, (1936) Bull. Geol. Soc. Amer., 47, 775-850, (137-150).

_____, (1945) In: Leake, B. E. (1968) op. cit., (139).

Bartholme, P. (1960) Econ. Geol., 55, 255-277, (140).

Batieva, I. D., & Belkov, I. V. (1953) In: Leake, B. E. (1968) op. cit., (141).

Bearth, P. (1959) Schweiz. miner. petrogr. Mitt., 39, 267-286, (142).

Beck, L. C. (1842) In: Weidman, S. (1903) Am. J. Sci., 15, 227-232, (2298).

Beer, K. E. (1952) In: Harker, R. I. (1963) J. Petrology, 3, 215-237, (795).

Belyankin, D. (1909) In: Grigoriev, D. P., & Ishull, E. W. (1937) Am. Miner., 22, 169-177, (706).

_____, (1910) In: Leake, B. E. (1968) op. cit., (146,147,537).

_____, & Donnay, E. V. (1941) Ibid., (140).

Bentley, R. D. Ibid., (149-153).

Berwerth, (1892) In: Boggild, O. B. (1905) Meddel. om Grönland, 32, (323).

Best, L. G., & Mercy, E. L. P. (1967) Am. Miner., 52, 436-474, (2751-2754).

Bestow, G. (1929) In: Leake, B. E. (1968), op. cit., (164,538,539).

Bhaskar, Rao B. (1963) Ibid., (165, 1787).

Bilgrami, S. A. (155) Mineral. Mag., 30, 633-644, (166,169,171, 173,175).

_____, (1964) In: Leake, B. E. (1968), (177).

_____, & Howie, R. A. (1960) Am. Miner., 45, 791-801, (178).

Billings, M. (1928) Ibid. 13, 287-296, (180,185).

_____, (1937) Bull. Geol. Soc. Amer., 48, 463-566, (188).

Binns, R. A. (1965a) Mineral. Mag., 34, 52-65, (2741-2750).

_____, (1965b) Ibid., 35, 306-326, (2367-2388).

_____, (1967) J. Petrology, 8, 349-371, (190).

_____, (1969) Am. J. Sci., 267A, 33-49, (192).

Black, P. M. (1970) Am. Miner., 55, 508-511, (193,194).

_____, (1970) Ibid., 55, 1061-1064, (195,196).

Blasdale, W. C. (1901) In: Leake, B. E. (1968) op. cit., (197,540).

Bloomfield, K. (1958) Ibid., (198).

Bloxam, T. W. (1955) Geol. Mag., 92, 329-337, (199).

_____, & Allen, J. B. (1960) Trans. Roy. Soc. Edinburgh, 64, 1-28, (558-561).

Blyth, F. G. H., & Lambert, R. St. J. (1970) Q. Jl. geol. Soc. Lond., 125, 543-555, (1015-1021).

Bodewig, (1876) In: Bearth, P. (1959) Schweiz. miner. petrogr. Litt., 39, 267-286, (143).

Bonnischen, B. (1969) Mineral. Soc. Amer. Spec. Paper, 2,

217-239, (562-585).

Bonsdorff, P. A. V. In: Harrington, B. J. (1903) Am. J. Sci., 15, 392-394, (880).

_____, In: Laitikari, A. (1921) Bull. comm. Geol. Finl., 54, 115, (1307).

_____, (1922) Ibid., (1303).

_____, & Lindewall, C. F. (1816) Ibid., (1306).

Borg, I. Y. (1967) Contr. Mineral. and Petrology, 15, 67-92, (204-212).

Borioni, A. (1965) In: Klein, C. Jr. (1968) J. Petrology, 9, 281-330, (1153,1154).

Boriscnko, L. F. (1967) Mineral. Mag., 36, 403-410, (213-220).

Borley, G. D. (1963) Ibid., 33, 358-376, (221-230).

_____, & Frost, M. T. (1963) Ibid., 33, 646-662, (239-248).

_____, Suddaby, P., & Scott, P. (1971) Contr. Mineral. and Petrology, 31, 102-114, (249-260).

Bose, M. K. (1963) Am. Miner., 48, 1405-1409, (269).

_____, (1964) Mineral. Mag., 33, 912-917, (270,271).

_____, Chakravarti, S., & Sarkar, A. (1971) Geol. Mag., 108, 273-280, (557).

Bowen, N. L., & Schairer, J. F. (1955) Am. Miner., 20, 543-551, (1014).

Boyd, F. R. (1970) Carnegie Inst. Year Book, 70, 138-142, (324).

Brammall, A. In: Leake, B. E. (1968) op. cit., (272-279).

Brewer, (1850) In: Weidman, S. (1903) Am. J. Sci., 15, 227-232, (2299).

Brezina, A. (1874) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (2098).

Brock, P. W. G., Gellatly, D. C., & Knorring, O. von (1964) Mineral. Mag., 33, 1057-1065, (280-281).

Brogger, W. C. (1890) In: Leake, B. E. (1968) op. cit., (282).

_____, (1934) Ibid., (283).

_____, (1935) Ibid., (284).

Brouss, R., & Ildefonse, J. P. (1970) Bull. Volcan., 34, 792-822, (2760).

Brown, E. H. (1967) Contr. Mineral. and Petrology, 14, 259-292, (285-288).

Brown, P. E. (1956) Geol. Mag., 93, 72-84, (289).

Crowmlow, A. H. (1961) Am. J. Sci., 259, 353-370, (292-298).

Dryhini, I., & Griffin, W. L. (1971) Contr. Mineral. and Petrology, 32, 112-125, (299-304).

Buddington, A. F. (1952) Am. J. Sci., Bowen Vol., 37-84, (305-311).

_____, & Leonard, B. F. (1953) Am. Miner., 38, 891-902, (312-318).

Buerger, M. J. (1927) Ibid., 12, 374-378, (319,320).

Bugge, J. A. W. (1943) Norges Geol. Undersok., 160, (2306).

Burns, D. J. (1966) Geol. Mag., 103, 19-35, (325-331).

Burns, R. G., & Greaves, C. (1971) Am. Miner., 56, 2011-2033, (2516-2521).

_____, & Prentice, F. J. (1968) Ibid., 53, 770-776, (2509-2511).

Butler, J. P. (1969) J. Petrology, 10, 56-101, (332-356).

Butler, J. R. (1953) Geochim. Cosmochim. Acta, 4, 157-178, (357).

Cahill, B. J. (1968) Mineral. Soc. I.M.A. (I.M.A. papers and proc. 5th gen. meeting Cambridge 1966), 199-203, (2662-2665).

Callegari, E., & Lonese, A. In: Leake, B. E. (1968) op cit., (358).

Cameron, M., & Gibbs, G. V. (1970) Carnegie Inst. Year Book, 69, 150-153, (2523-2524).

Campbell, I., & Schenk, E. T. (1950) Am. Miner., 35, 671-692,

(358).

Card, K. D. (1964) Bull. Geol. Soc. Amer., 75, 1011-1030, (360).

Carmichael, I. S. E. (1967) Contr. Mineral. and Petrology, 14, 36-64, (366-374).

_____, (1967) Ibid., 15, 24-26, (365-368).

_____, (1970) J. Petrology, 11, 147-181, (361-364).

Carstens, C. W. (1918) In: Leake, B. E. (1968) op. cit., (375).

_____,(1920) In: Sundius, N. (1931) Am. J. Sci., 21, 330-344, (2151).

Cesaro, C. (1896) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (2683).

Challis, G. A. (1965) J. Petrology, 6, 395-419, (376-380).

Chesnokov, B. V. (1960) Intern. Geology, Rev., 2, 936-945, (2789-2790).

Chester, A. N., & Cairns, F. I. (1887) In: Peacock, M. A. (1928) Am. Miner., 13, 241-266, (1611,1612).

Chistalov, V. K. (1959) In: Leake, B. E. (1968) op. cit., (381,541,542).

Choudhuri, A., & Winkler, H. G. F. (1967) Contr. Mineral. and Petrology, 14, 293-315, (382).

Chrustchoff, (1891) In: Ford, W. A. (1914) Am. J. Sci., 37, 179-193, (672).

Clarke, F. W. (1900) In; Leake, B. E. (1968) op. cit., (383).

_____,(1910) Ibid., (384,543-545).

Coleman, R. G. (1951) Bull. Geol. Soc. Amer., 62, 1517, (757).

_____, Lee, D. E., Beatty, L. B., & Brannock, W. W. (1965) Ibid., 76, 483-508, (385).

_____, & Papike, J. J. (1968) J. Petrology, 9, 105-128, (387-401).

Collins, R. S. (1942) Mineral. Mag., 26, 254-259, (386, 402,403).

Comeferro, J. E., & Kohn, J. A. (1954) Am. Miner., 39, 537-548, (404).

Compton, R. R. (1958) Ibid., 43, 890-907, (405-409).

Conquere, F. (1971) Contr. Mineral. and Petrology, 30, 296-313, (410-412).

_____, (1971) Ibid., 33, 32-61, (2398-2404).

Conyat, J. (1908) In: Leake, B. E. (1968) op. cit., (424).

Cooper, A. F. (1971) Bull. Geol. Soc. Amer., 82, 1327-1339, (413).

_____, (1972) J. Petrology, 13, 457-492, (2589-2591).

_____, & Lovering, J. F. (1970) Contr. Mineral. and Petrology, 27, 11-24, (414-423).

D'Achiardi, G. (1912) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1811).

D'Cruz, J., Nagenna, C., & Sadashivaiah, T. S. (1958) In: Leake, B. E. (1968) op. cit., (425).

Daly, R. A. (1899) Ibid., (426).

Daniels, J. L. (1956) Ibid., (427,546-548).

Das Gupta, S. P. (1967) Mineral. Mag., 36, 22-28, (430).

Davidson, C. F. (1943) Trans. Roy. Soc. Edinburgh, 61, 75, (2434-2435).

Dearnley, R. (1963) Q. Jl. Geol. Soc. Lond., 119, 243-312, (428-429).

Deer, W. A. (1938) Mineral. Mag., 25, 56-74, (431-439).

_____, Howie, R. A., & Zussman, J. (1963) In: Aoki, K. (1964) Am. Miner., 49, 1199-1223, (50).

Des Cloiszeux, A. (1861) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1812).

_____, (1862) Ibid., (1813).

_____, (1867) In: Boggild, O. B. (1905) Meddel. om Grönland, 32, (203).

_____, (1868) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1814).

Dickey, J. S. (1968) Am. Miner., 53, 1304-1319, (440).

Dimanche, F. (1970) Bull. Soc.fr. Miner. Crystallogr., 53, 89-100, (2767-2772).

Dodge, F. C. W., Popike, J. J., & Hays, R. E. (1968)
J. Petrology, 9, 378-410, (441-460).

_____, & Ross, D. C. (1971) J. Geol., 79, 158-172,
(549-556).

Doelter, C. (1888) In: Peacock, M. A. (1928) Am. Miner., 13,
241-286, (460).

_____, (1914) In: Leake, B. E. (1968) op. cit., (461).

Dolar, Mantuani, L., Gagarin, C. (1936) Ibid., (462).

Drysdall, A. R., Newton, A. R. (1960) Am. Miner., 45, 53-59,
(482,483).

Dufrenoy, A. (1836) In: Rabbit , J. C. (1948) Am. Miner.,
33, 263-323, (1966).

Dunn, J. A., & Roy, P. C. (1938) In: Pilgrami, S. A. (1955)
Mineral. Mag., 30, 633-644, (170).

Duparc, L., & Hormung, J. G. (1907) In: Leake, B. E. (1968)
op. cit., (463-472).

_____, & Pearce, F. (1903) Ibid., (473,474,675).

_____, _____, (1908) Ibid., (475).

Du Rietz, T. (1929) Ibid., (476).

_____, (1935) Ibid., (478,479).

_____, (1938) Ibid., (480,481).

Eakins, L. G. (1890) Ibid., (490).

Edelman, N. (1960) Ibid., (491).

Edwards, A. B. (1938) Q. Jl. Geol. Soc. Lond., 94, 243-318, (492).

_____, (1950) In: Leake, B. E. (1968) op. cit.,
(493-496).

_____, Baker, G., & Callow, M. J. (1956) Ibid., (497).

Efremov, N. E. (1938) Ibid., (498).

Eggler, D. H. (1972) Earth Planet. Sci. Letters, 15, 28-34,
(2668-2669).

Eggleston, J. T. (1918) In: Billings, . . (1928) Am. Miner.,
13, 287-296, (192).

Engel, A. E. J., & Engel, C. G. (1962) Bull. Geol. Soc. Amer., 73, 1499-1514, (489-532).

Engel, C. G. (1959) Ibid., 70, 951-980, (586-591).

Erdmannsdorffer, T. H. (1929) In: Leake, B. E. (1968), (592).

_____, (1935) Ibid., (593-594).

Erlank, A. J., & Finger, L. W. (1970) Carnegie Inst. Year Book, 68, 320-324, (2040-2042).

Ernst, W. G. (1960) Geochim. Cosmochim. Acta., 19, 10-40, (595).

_____, (1963) Am. Miner., 48, 241-260, (596).

_____, (1964) Geochim. Cosmochim. Acta, 28, 1631-1668, (597-599).

_____, (1966) Am. J. Sci., 264, 37-65, (763).

_____, (1972) Mem. Geol. Soc. Amer., 135, 73-94, (2843-2851).

_____, Seki, Y., Onuki, H., & Gilbert, M. C. (1970) Mem. Geol. Soc. Amer., 124, (2812-2825).

_____, & Wai, C. M. (1970) Am. Miner., 55, 1226-1258, (603-605).

Eskola, P. (1914) Bull. comm. geol. Finl., 40, (607, 609-611, 613).

_____, (1915) Ibid., 44, (618-625).

_____, (1921) In: Alderman, A. R. (1936) Q. Jl. geol. Soc. Lond., 92, 488-530, (3).

_____, (1925) In: Leake, B. E. (1968) op. cit., (626).

_____, (1936) Bull. comm. geol. Finl., 115, (627-630).

_____, (1952) Am. J. Sci., Bowen Vol., 133-171, (631).

_____, & Mervinen, T. (1936) Bull. comm. geol. Finl., 115, 475-487, (1155, 1156).

_____, & Sahlstein, G. (1930) Ibid., 92, 77, (632).

Evans, F. F., & Bancroft, J. A. (1908) Am. J. Sci., 26, 509-512, (636).

Ewart, A. (1965) In: Leake, B. E. (1968) op. cit., (638).

_____, (1971) In: Buckley, A. F., & Wilkins, R. W. T. (1971)

Am. Miner., 56, 90-100, (302).

Fabries, J. (1969) In: Leake, B. E. (1968) op. cit., (659-650).

_____, (1968) Mineral. Soc. I.M.A. (I.M.A. papers and proc. 5th Gen. Meeting, Cambridge 1966), 204-211, (650-661).

Fahlquist, F. (1910) In: Leake, B. E. (1968) op. cit., (710).

Favorskaya, M. A. (1946) Ibid., (651).

Fedoseev, A. D., Grigoreva, L.F., Chigareva, O. G., & Romanov, D. P. (1970) Am. Miner., 55, 854-863, (652-662).

Fermor, L. L. (1909) In: Leake, B. E. (1968) op. cit., (167,663).

Ficke, B. (1960) Tschermaks miner. petrogr. Mitt., 7, 337-436, (664).

Finger, L. W. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 95-100, (2505).

_____, (1970) Am. Miner., 55, 300, (2506).

Finlayson, A. M. (1909) Q. Jl. geol. Soc. Lond., 65, 351-381, (665).

Finucane, M. J. (1939) In: Drysdall, A. R., & Newton, A. R. (1960) Am. Miner., 45, 53-59, (484,485).

Fletcher, C. J. N. (1971) Can. J. Earth Sci., 8, 1065-1080, (666,667).

Forbes, W. C. (1971) Am. Miner., 56, 997-1004, (668).

Ford, W. E. (1914) Am. J. Sci., 37, 179-193, (1721-1730).

Forestier, F. H. & Lasnier, M. (1969) Contr. Mineral. and Petrology, 23, 194-235. (674-681).

Foshag, W. F. (1936) Am. Miner., 21, 63-67, (682).

Foslie, S. (1945) In: Leake, B. E. (1968) op. cit., (683-689).

Fougue, J. A. (1902) Ibid., (690).

Francis, G. H. (1955) Mineral. Mag., 30, 709-716, (691).

_____, (1958) Geol. Mag., 95, 25-39, (692).

_____, (1958) Brit. Mus. Nat. Hist. (Mineralogy), 1,

121-162, (603-635).

Franco, S. Di (1915) In: Leake, B. E. (1968) op. cit., (606).

Frankel, J. J. (1944) Ibid., (607).

Frosth, S. J. (1965) Ibid., (691,692).

Freudenberg, W. (1908) In Frider, R. V. (1959) Mineral. Mag., 25, 373-387, (1771).

Frey, M. (1969) In: Leake, B. E. (1971) Mineral. Mag., 38, 389-407, (2809).

Friedel, C. (1902) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1808).

Frisch, T. (1970) Can. Mineral., 10, 553-570, (2406-2418).

_____, & Schminche, H. U. (1969) Bull. Volcan., 33, 1073-1088, (2405).

Frost, M. T. (1963) Mineral. Mag., 33, 377-384, (709-717).

Frosterus, B. J., & Wilkman, W. W. (1924) In: Vahatalo, V. C. (1953) Bull. comm. geol. Finl., 164, 42, (2199).

Gabinet, M. P. (1951) In: Leake, B. E. (1968) op. cit., (718).

Galkin, N. (1910) Ibid., (721-727).

Gallaher, M. J. (1963) Mineral. Mag., 33, 415-430, (720).

Garson, M. S. (1960) In: Smith, W. C., et al. (1960) Mineral. Mag., 36, 1164-1167, (2005).

Gavolin, S. (1933) In: Leake, B. E. (1968) op. cit., (728).

Geijer, P. (1913) Ibid., (728,730).

Genth, F. A. (1882) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1817).

Ghent, E. D., & DeVries, D. S. (1972) Can. J. Earth Sci., 9, 618-635, (2675-2680).

Ghose, S. (1961) Acta Crystallogr, 14, 622-627, (2504).

_____, & Hollner, H. (1959) J. Geol., 67, 691-701, (2507).

_____, & Weidner, J. R. (1971) Contr. Mineral. and Petrology, 30, 64-71, (731).

Gibbs, G. V. (1969) Mineral. Soc. Amer. Spec. Paper, 2,

101-109, (2388).

_____, & Miller, J. L., & Shell, E. R. (1962) Am. Miner., 47, 75-82, (752).

Giesecke, (1810) In: Boggild, O. B. (1905) Meddel. om Gronland, 32, (200).

Gilbert, M. C. (1966) Am. J. Sci., 264, 698-742, (733).

Ginzburg, I. V., & Ognolodkina, G. A. (1966) In: Cerny, P. (1968) Neues Jb. Miner. Mb., 57-61, (2272).

_____, Yukhenvich, G. V., Persman, A. B., & Vernadskii, V. I. (1962) Geochemistry Ann. Arbor., 31-38, (734-740).

Gjelsvik, T. (1947) In: Leake, B. E. (1968) op. cit., (741).

Glagolev, A. A., & Klaguish, B. D. (1959) Ibid., (742-744).

Gmelin, C. G. (1816) In: Laitikari, A. (1921) Bull. comm. geol. Finl., 54, 113, (1305).

Gnativ, G. M. (1959) In: Leake, B. E. (1968) op. cit., (745).

Goroshnilov, V. I., & Yuryev, L. D. (1965) In: Nisch, M. J. (1969) Contr. Mineral. and Petrology, 21, 319-331, (1049).

Gottried, C. (1929) In: Leake, B. E. (1968) op. cit., (746).

Goltz, J. (1884) In: Hall, A. (1930) Geol. Surv. S. Africa, 32, (701).

Grant, J. A., Weiblen, P. W. (1971) Am. J. Sci., 270, 281-296, (2358).

Green, D. H. (1964) J. Petrology, 5, 134-188, (747,748).

_____, (1964) J. Geol., 72, 543-563, (749-752).

_____, & Hysen, B. O. (1972) Lithos, 5, 147-161, (2601-2606).

Greenwood, H. J. (1963) J. Petrology, 4, 317-351, (753).

Greenwood, R. (1951) Bull. Geol. Soc. Amer., 62, 1151-1178, (754).

Griffin, W. L. (1971) J. Petrology, 12, 219-243, (2708-2710).

_____, & Heier, K. S. (1969) Contr. Mineral. and Petrology, 23, 89-116, (755).

Grigorjeva, R. F., Chigorjova, C. G., & Fedoseev, A. D. (1967)

The Physics and Chemistry of the Asbestiform Minerals, Oxford, 1967, (2775-2792).

Groves, A. W. (1935) Q. Jl. geol. Soc. Lond., 91, 150-204, (758,759).

Gubelin, E. (1939) Schweiz. miner. petrogr. Mitt., 19, 325-442, (760).

Gulson, B. L., Lovering, J. F., Taylor, S. R., & White, A. J. R. (1972) Lithos, 5, 269-279, (2598-2600).

Gruner, E. L. (1848) In: Warren, H. V. (1931) Mineral. Mag., 22, 477-481, (2251).

Guitard, G. & Lafitte, P. (1968) In: Leake, B. E. (1968). op. cit., (761).

Gumbel, C. W. V. (1891) Ibid., (762).

Gunn, B. M. (1972) Can. Mineral., 11, 840-850, (2598).

Guppy, E. M., Sabine, P. A. (1956) Mem. Geol. Surv. U. K., 78pp, (764-767).

_____, Thomas, H. H., & Ennos, F. R. (1951) Ibid., 166pp, (768,769).

Gupta, J. P. das (1972) Mineral. Mag., 38, 890-893, (2580,2581).

Gustavson, M., & Gronhaug, A. (1959) In: Leake, B. E. (1968) op. cit., (770).

Gutberlett, H. G., & Huckenholz, H. G. (1965) Ibid., (771).

Haapla, P. (1936) Bull. comm. geol. Finl., 114, 88, (1819-1822).

Haefcke, H. (1893) In: Leake, B. E. (1968) op. cit., (772-775).

Hagner, A. F., Leung, S. S., & Dennison, J. M. (1965) Am. Miner., 50, 314-355, (776-780).

Hall, A. (1930) In: Drysdall, A. R., & Newton, A. R. (1960) Am. Miner., 45, 53-59. (486,487).

Hallimond, A. F. (1947) Am. Miner., 28, 230-243, (788).

Harada, Z. (1942) In: Leake, B. E. (1968) op. cit., (789).

Haramura, F. (1963) Ibid., (790,791).

Harbrich, E. (1929) Ibid., (792).

Harker, R. I. (1963) J. Petrology, 3, 215-237, (793,794).

Harrington, B. J. (1903) Am. J. Sci., 15, 392-394, (796-798).

Harris, R. L. Jr. (1959) Bull. Geol. Soc. Amer., 70, 1185-1216, (801-803).

Harry, W. T. (1951) Q. Jl. Geol. Soc. Lond., 107, 137-156, (804).

Harumoto, A. (1955) In: Aoki, A. (1963) J. Petrology, 4, 198-210, (38).

Hashimoto, A. (1961) In: Leake, B. E. (1968) op. cit., (805,806).

Hashimoto, I. (1968) J. Fac. Sci. Tokyo Univ., 17, 100-162, (807-809).

Haslam, H. W. (1968) J. Petrology, 9, 84-104, (810-820).

_____, (1970) Geol. Mag., 107, 341-356, (822,821).

_____, & Walker, B. G. (1971) Mineral. Mag., 38, 58-63, (2359-2362).

Hasler, P. (1949) Schweiz. miner. petrogr. Mitt., 29, 50-152, (823).

Hausmann, & Stromeyer, (1831) in; Peacock, M. A. (1928) Am. Miner., 13, 241-286, (1687,1689).

Hayama, Y. (1964) Jap. J. Geol. Geogr., 35, 193-204, (824-826).

Heddle, M. F. (1879) Mineral. Mag., 2, 9-35, (1756).

Heflik, W. (1964) In: Leake, B. E. (1968) op. cit., (827,828).

Heier, K. (1961) Norsk. geol. tidsskr., 41, 109-155, (829).

Heimlich, R. A. (1965) Bull. Geol. Soc. Amer., 76, 1-26, (830-831).

_____, (1971) Geol. Mag., 108, 1-12, (2737,2738).

Heinrich, E. W. (1965) Am. Miner., 48, 597-613, (836,837).

Henderson, C. M. B. (1968) Mineral. Soc. I.M.A. (I.M.A. papers and proc. 5th gen. meeting, Cambridge 1966), 291-304, (966-978).

Henderson, E. P. (1931) Am. Miner., 16, 563, (838).

Henry, N. F. M. In: Leake, B. E. (1968) op. cit., (839).

Heritsch, H. (1965) Tschermaks miner. petrogr. Mitt., 10, 209-217, (840).

_____, Bertoldi, G., & Walitzi, E. M. (1960) Ibid.,

7, 210-217, (841).

_____, & Kohler, E. (1960) Ibid., 7, 218-234, (843,844).

_____, Paulitsch, P., & Walitzi, E. F. (1957) Ibid., 6, 215-225, (845,846).

_____, & Reichert, (1960) Ibid., 7, 253-245, (847).

Hermes, C. D. (1970) Bull. Geol. Soc. Amer., 81, 157-161, (848-867).

Heron, A. . (1924) In: Leake, B. E. (1968) op. cit., (868).

Hezner, L. (1903) Ibid., (832).

_____, (1908) Ibid., (835-865).

Hietanen, A. (1938) Bull. comm. geol. Finl., 122, (870-872).

_____, (1959) Am. Miner., 44, 539-564, (873).

_____, (1963) In: Leake, B. E. (1968) op. cit., (874,875).

_____, (1971) Contr. Mineral. and Petrology, 30, 161-176, (876-880).

_____, (1971) Am. Miner., 56, 234-239, (881).

Hillebrand, S. (1908) In: Leake, B. E. (1968) op. cit., (882).

Himmelberg, G. R., & Papike, J. J. (1969) J. Petrology, 10, 102-114, (2824-2831).

Hinds, H. E. A. (1921) Am. J. Sci., 1, 355-364, (883-885).

Hisinger, W. (1818) In: Laitikari, A. (1921) Bull. comm. geol. Finl., 54, 113, (1302).

HLa, T. (1945) Mineral. Mag., 27, 137-146, (886,887)

Hodgson, A. A. (1965) Ibid., 35, 291, (888-903).

Hoffman, C. (1970) Contr. Mineral. and Petrology, 27, 283-320, (904-907).

_____, (1972) Ibid., 34, 135-149, (2392,2393).

Hofman, F. (1964) In: Leake, B. E. op. cit., (908).

Holdaway, M. J. (1965) Am. Miner., 50, 993-977, (909-918).

Holgate, N. (1951) Mineral. Mag., 29, 792-798, (919).

Hollander, H. E. (1970) Lithos, 3, 93-111. (921-937).

Holloway, J. R., & Burnham, C. W. (1972) J. Petrology, 13, 1-29, (2661-2667).

Holm, E. F. (1972) Am. Miner., 56, 2111, (938-940).

Nolser, W. T. (1950) Bull. Geol. Soc. Amer., 61, 1053-1090, (941-942).

Normung, G., & Knorring, C. von (1962) Trans, Geol. Soc. S. Africa, 65, 153-180, (943).

Howie, R. A. (1955) Trans. Roy. Soc. Edinburgh, 62, 725-768, (2425-2429).

———————, (1963) Mineral. Mag., 33, 718-719, (944,945).

———————, (1964) Science Progress, 52, 637, (2430).

Huebner, J. S., & Papike, J. J. (1970) Am. Miner., 55, 1973-1992, (946-949).

Hutton, C. O. (1938) Mineral. Mag., 25, 207-211, (979).

———————, (1956) Acta Crystallogr., 9, 231-232, (980).

Hytonen, K. (1959) Bull. comm. geol. Finl., 184, 75-131, (981).

Ichimura, T. (1931) Mineral. Mag., 22, 561-568, (982,983).

Ishii, I., & Yamada, T. (1962) In: Leake, B. E. (1968) op. cit., (984-988).

Ishyul, V. (1917) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1002).

Ivanov, I. P., & Sidorenko, G. A. (1965) In: Leake, B. E. (1968) op. cit., (989,990).

Iwasaki, M. (1960) In: Ernst, W. G. (1963) Geochim. Cosmochim. Acta, 28, 1631-1668, (601,602,991).

Jaffe, H. W., Groeneveld, Meijer, W. O. J., & Selchow, D. H. (1961) Am. Miner., 46, 642-653, (992).

Jakob, J. (1927) Schweiz. miner. petrogr. Mitt., 7, 137-139, (993-995).

———————, (1935) Ibid., (996-1000).

Jambor, J. L. (1971) Can. Mineral., 11, 34-75, (2673,2674).

Janowsky, (1875) In: Boggild, O. B. (1905) Meddel. om Gronland, 32, (202).

Jons, H., & Bethune, P. De (1968) Mineral. Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting, Cambridge 1966) 312-314, (1013).

Jayaraman, V. (1940) In: Leake, B. E. (1968) op. cit., (1001-1002).

Jimbo, K. (1926) Ibid., (1003,1004).

Johansson, K. (1930) In: Sundius, N. (1931) Am. J. Sci., 21, 330-344, (2150).

John, J. F. (1809) In: Rabbit , J. C. (1940) Am. Miner., 33, 263-323, (2095).

Johnson, E. L., & Warren, C. F. (1940) Am. J. Sci., 25, 1-38, (1005).

Jones, W. A. (1930) Contr. Canadian Mineralogy, 61-73, (1006).

Jung, J. (1927) In: Leake, B. E. (1968) op. cit., (1007).

Jure, A. E. (1930) Ibid., (1008-1012).

Kaiser, F. In: Hall, A. (1930) Geol. Surv. S. Africa, 32, p.310, (786,787).

_____, (1925) In: Leake, B. E. (1968) op. cit., (1022).

Kalsbeek, F. (1962) Ibid., (1023-1027).

Kanisawa, S. (1964) Ibid., (1028-1031).

Kardymowicz, I. (1957) Ibid., (1032).

Kaufman, H. (1963) Ibid., (1033-1039).

Kawano, Y. (1934) In: Aoki, K. (1963) J. Petrology, 4, 198-210. (41)

Kempe, D. R. C. (1968) Mineral. Mag., 36, 874-876, (1040).

_____, (1968) Ibid., 1167-1169, (1041).

Kennedy, W. Q., & Dixon, B. E. (1936) In: Leake, B. E. (1968) op. cit., (1042).

Keyser, F. De (1966) Contr. Mineral. and Petrology, 12, 315-324, (1043-1044).

Kisch, H. J. (1969) Ibid., 21, 319-331, (1045-1046).

_____, & Warnaars, F. W. (1969) Ibid., 24, 245-267, (1050-1069).

Klaproth, M. H. (1915) In: Peacock, M. A. (1928) Am. Miner., 13, 241-286, (1686).

Klein, C. Jr. (1966) Am. Miner., 49, 963-982, (1070-1078).

_____, (1968) J. Petrology, 7, 246-305, (2555-2562).

_____, (1968) Ibid., 9, 281-330, (1079-1152).

———————, (1969) Am. Miner., 54, 212-237, (1155-1176,1179-1200).

———————, & Ito, J. (1968) Ibid., 53, 1264-1275, (1201-1213).

Klemm, G. (1895) In: Leake, B. E. (1968) op. cit., (1214, 1215).

Klerks, J. (1964) Ibid., (1216).

Knofel, D., Englehardt, W. V. (1964) Ibid., (1217,1218).

Knorring, O. von, & Hornung, G. (1961) Mineral. Mag., 32, 731-735, (1219-1220).

———————, & Kennedy, W. Q. (1958) Ibid., 31, 846-859, (1221).

Kohn, J. M., & Comeferro, J. E. (1955) Am. Miner., 40, 410-421, (1222-1224).

Koike, S. (1925) In: Leake, B. E. (1968) op. cit., (1225).

Kolderup, N. H. (1925) Ibid., (1226,1227).

Konig, A. (1927) In: Bain, A. D. M. (1934) Q. Jl. geol. soc. Lond., 90, 201-236, (91).

Koritnig, S. (1940) In: Binns, R. A. (1967) J. Petrology, 8, 349-371, (191).

Korjinsky, D. S. (1945) In: Leake, B. E. (1968) op. cit., (1228-1230).

Kornilow, F. A. (1959) Ibid., (1231-1233).

Korytkova, E. N., Fedoseyev, A. D., & Makarova, T. A. (1968) Dokl. Acad. Sci. USSR Earth Sci. Sect., 182, 145-147, (2271).

Korzhinsky, A. F. (1956) In: Leake, B. E. (1968) op. cit., (1234-1244).

Kovalenko, V. I. (1968) Mineral. Soc. I. M. A. vol. (I.M.A. papers and proc. 5th gen. meeting, Cambridge, 1966), 261-284, (2488-2493).

Kowalski, W. M., & Oszacka, B. (1964) In: Leake, B. E. (1968) op. cit., (1245).

Kozu, S., & Kawano, Y. (1940) Ibid., (1246).

———————, Yagi, T., & Kani, K. (1929) Ibid., (1247).

Krank, S. F. (1961) J. Petrology, 3, 137-184, (1248-1255).

Krenner, J. A. (1899) In: Ford, W. E. (1914) Am. J. Sci., 37, 179-193, (671).

_____, (1900) In: Leake, B. E. (1968) op. cit., (1256).

Kretz, R. (1959) J. Geol., 67, 371-402, (1257-1272).

Kroutz, S. (1908) In: Leake, B. E. (1968) op. cit., (669,670, 1273-1282).

Kroustchoff, K. De (1891) In: Halser, W. T. (1950) Bull. Geol. Soc. Amer., 61, 1053-1090, (942).

Krutov, G. A. (1936) In: Leake, B. E. (1968) op cit., (1283).

Kuchler, H. (1914) Ibid., (1284,1285).

Kukouski, E. G. (1950) Ibid., (1286).

Kulling, O. (1933) Ibid., (1287).

Kunitz, W. (1930) In: Bearth, P. (1959) Schweiz. miner. petrogr. Mitt., 39, 267-286, (145).

Kuroda, Y. (1959) In: Leake, B. E. (1968) op. cit., (1288-1293).

Lacroix, A. (1904) Ibid., (1294).

_____, (1907) Ibid., (1295).

_____, (1910) In: Bilgrami, A. (1955) Mineral. Mag., 30, 633-644, (168).

_____, (1939) In: Leake, B. E. (1968) op. cit., (1296).

Ladieva, V. D. (1956) Ibid., (1297).

Laitikari, A. (1920) Bull. comm. geol. Finl., 54, (1298-1301).

Lal, R. K. (1969) Lithos, 2, 187-196, (1308,1309).

Lappe, L. (1835) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (2100).

Larsen, E. S. (1938) Am. J. Sci., 35, 94-103,(1310-1326).

_____, (1942) U. S. Geol. Surv. Prof. Paper, 197, (2832-2836).

_____, & Draisen, W. M. (1948) International Geol. Congress 18th Session Great Britain, Pt. 2, 66-79, (1327-1337).

_____, & Irving, J. (1937) Am. Miner., 22, 889-905, (1338-1340).

Landermilk, J. D., & Woodford, A. C. (1950) Ibid., 15, 259-262, (1341).

Laughlin, A. W., Brookins, D. G., Rudo, A. N., & Causey, J. D. (1971) Geochim. Cosmochim. Acta, 35, 107-113, (1342).

Lavisto, D. (1915) In: Leake, B. E. (1968) op. cit., (1343).

Lemaitre, R. W. (1969) Mineral. Mag., 37, 185-197, (2717,2718).

Leake, B. E. (1962) Jap. J. Geol. Geogr., 33, 1-13, (1344-1348).

_____, (1965) Am. Miner., 50, 843-851, (1350-1352).

_____, (1971) Mineral. Mag., 38, 389-407, (2805-2806).

_____, (1972) Ibid., 38, 649-665, (2593-2598).

Lebedinsky, V. I. (1952) In: Leake, B. E. (1968) op. cit., (1353).

Lee, T. W. et.al. (1966) In: Klein, C. Jr. (1969) Am. Miner., 54, 212-257, (1177,1178).

Leeds, A. R. (1873) Am. J. Sci., 9, 229-230, (2093,2094).

Leelandam, C. (1970) J. Petrology, 11, 475-505, (1354-1362).

Lensch, G. (1971) Contr. Mineral. and Petrology, 31, 145-153, (1363).

Leveson, D. J. (1963) Bull. Geol. Soc. Amer., 74, 1015-1040, (1364-1366).

Levin, S. B. (1950) Ibid., 61, 519-565, (1367).

Lewis, J. V. (1896) In; Leake, B. E. (1968) op. cit., (1368).

Lindgren, W., & Melville, W. H. (1893) Ibid., (1997).

Lindroth, G. T. (1922) Ibid., (1369).

Linthout, K., & Kieft, C. (1970) Mineral. Mag., 37, 629-631, (2719).

Lipman, P. W. (1964) Am. Miner ., 49, 1321-1330, (1370-1372).

Litvin, A. L. (1964) In: Leake, B. E. (1968) op. cit., (1373-1381).

Livingstone, A. (1967) Mineral. Mag., 36, 380-387, (1382).

Loewinson-Lessing, F. (1900) In: Leake, B. E. (1968) op. cit., (1383).

Lokka, L. (1950) Bull. comm. geol. Finl., 149, (1384).

Lord, F. C. F. (1890) In: Billings, L. (1938) Am. Miner., 13, 287-296,

Lorenzen, J. (1884) In: Washington, H. S. (1908) Am. J. Sci., 25, 107-211, (2254).

_____, Meddel. om Gronland, 2, 45-79, (1385-1387).

Lovering, J. F., & White, A. J. R. (1969) Contr. Mineral. and Petrology, 21, 9-52, (1388-1393).

Lowder, G. G. (1970) Ibid., 26, 324-340, (1394-1396).

Lukac, R. (1934) In: Leake, B. E. (1968) op. cit., (1397).

_____, (1935) Ibid., (1398-1400).

Lundergardh, P. H. (1943) Ibid., (1401,1402).

Lundquist, T. (1962) In: Akella, J., & Winkler, H. G. F., (1966) Contr. Mineral. and Petrology, 12, 1-12, (1).

Lupanova, N. P. (1934) In: Leake, B. E. (1968) op. cit., (1403).

Lutts, B. G. (1962) Ibid., (1404-1407).

_____, (1969) Geochemistry International, 6, 624-629, (2394).

Lyons, P. C. (1972) Am. Miner., 57, 1404-1412, (2583-2586).

McKee, D. (1963) Mineral. Mag., 33, 635-645, (1408).

Mclachlan, G. R. (1951) Ibid., 29, 477-495, (1409).

Machatschki, F., & Walitzi, E. F. (1963) Tschermaks miner. petrogr. Mitt., 8, 140-151, (1410-1414).

Maciejewski, St. (1954) In: Leake, B. E. (1968) op. cit., (1417).

Mackay, R. A., Greenwood, R., & Rockingham, J. E. (1949) Bull. Geol. Surv. Nigeria, 19, (1415).

Mackenzie, D. B. (1960) Bull. Geol. Soc. Amer., 71, 303-318, (1416).

Magnusson, N. H. (1930) In: Leake, B. E. (1968) op. cit., (1772).

_____, (1940) Ibid., (1418-1420).

Majmundar, H. H. (1969) Can. Mineral., 10, 97-100, (1423-1425).

Makarova, T. A., Kortkova, E. V., & Fedoseev, A. D. (1967) Physics and Chemistry of the Asbestiform Minerals, Oxford,

(2703-2707).

Makinen, E. (1915) In: Leake, B. E. (1968) op. cit., (1426).

Makuklina, G. O. (1960) Ibid., (1427-1430).

Marakushev, A. A., & Polin, Y. K. (1961) Geochemistry, 204-207, (2762).

Marchet, A. (1925) In: Leake, B. E. (1968) op. cit., (1431,1432).

Marshall, P. (1906) Q. Jl. Geol. Soc. Lond., 62, 381-424, (1433).

Marmo, V. (1960) Bull. comm. geol. Finl., 190, (1434)

Marx, V. A. (1962) In: Leake, B. E. (1968) op. cit., (1435,1436).

Mason, B. (1953) Am. Miner., 38, 862-865, (1437).

_____, (1966) In: Philpotts et al. (1972) Geochim. Cosmochim. Acta, 36, 1131-1166, (2765).

_____, (1968) Mineral. Mag., 36, 997-1002, (1438-1444).

Mathews, D. W. (1967) Scott. J. Geol., 3, 17-33, (1445).

Mathias, M. (1952) Trans. Geol. Soc. S. Africa, 55, 13-18, (1446,1447).

Mathur, K. K., Jhingran, H. G. (1931) In: Leake, B. E. (1968) op. cit., (1448).

Matlorsky, C. I. (1960) Ibid., (1449).

Matsumoto, H. (1954) Ibid., (1450).

_____, (1956) Ibid., (1451).

_____, (1963) Ibid., (1452).

Matsumoto, Y., & Miyashiro, H. (1960) Ibid., (1453).

Mauritz, B. (1911) Ibid., (1454).

Meng, H. H., & Chang, K. (1933) Ibid., (1455).

Merlainen, K. (1961) Bull. comm. geol. Finl., 195, (1456-1458).

Merwin, H. E., Washington, H. S. (1923) Am. Miner., 8, 63-67, (1459).

Metz, A. (1957) In: Leake, B. E. (1968) op. cit., (1460).

Meyer, H. O. A., & Brookins, D. G. (1971) Contr. Mineral. and Petrology, 34, 60-72, (2395).

Michaelson, A. (1863) In: Eskola, P. (1914) Bull. comm. geol.

Finl., 40, (616).

Mikkola, A. (1949) Bull. comm. geol. Finl., 146, (1461).

Mikkola, E., & Sahama, T. G. (1936) Ibid., 115, 357-371, (1462).

Miles, K. R. (1943) Am. Miner., 28, 25-38, (1463).

Milton, D. J., & Ito, J. (1961) Ibid., 46, 734-740, (1464).

Miyake, T. (1947) In: Leake, B. E. (1968) op. cit., (1465).

Miyashiro, A. (1953) Jap. J. Geol. Geogr., 23, 82-107, (1466,1467).

_____, (1958) J. Fac. Sci. Tokyo Univ., 11, 219-272, (1468,1469).

_____, & Iwasaki, I. (1957) J. Geol. Soc. Japan, 63, 698-703, (600).

_____, & Miyashiro, T. (1956) In: Aoki, K. (1964) Am. Miner., 49, 1199-1223, (52).

Noberg, A. (1956) In: Laitakari, A. (1921) Bull. comm. geol. Finl., 54, 113, (1307).

Nonchoum, P. (1972) Contr. Mineral. and Petrology, 37, 47-64, (2670-2672).

Moore, P. B. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 111-115, (2525).

Morgan, B. A. (1970) J. Petrology, 11, 101-145, (1470-1478).

Morkovkina, V. F. (1953) In: Leake, B. E. (1968) op. cit., (1479,1480).

Morozewicz, J. (1903) Ibid., (1481).

_____, (1925) In: Eskola, P., & Sahlstein, L. (1930) Bull. comm. geol. Finl., 92, 77-95, (634,635).

_____, (1925) In: Leake, B. E. (1968) op. cit., (1487,1488).

_____, (1926) Ibid., (1481-1485).

_____, (1928) Ibid., (1486).

Mottana, A., Church, W. R., & Edgar, A. D. (1968) Contr. Mineral. and Petrology, 18, 338-346, (2397).

Mottana, A., & Edgar, A. D. (1970) Lithos, 3, 37-49, (1490-1498).

Mueller, R. F., (1960) Am. J. Sci., 258, 449-497, (1492-1553).

Murakami, T., & Matsuo, E. (1963) In: Leake, B. E. (1968) op. cit., (1554).

Murty, N. S. (1961) Ibid., (1555).

_____, (1962) Ibid., (1556).

Nagasawa, H., & Schnetzler, C. C. (1971) Geochim. Cosmochim. Acta, 35, 953-968, (1557,1558).

Naidu, N. G. (1949) In: Leake, B. E. (1968) op. cit., (1559-1562).

_____, (1953) Ibid., (1563).

Naidu, P. R. J. (1942) Ibid., (1564).

_____, (1954) Ibid., (1565,1566).

_____, (1960) Ibid., (1567-1571).

Naik, M. S. (1963) Ibid., (1572,1573).

Nash, W. P., Carmichael, I. S. E., & Johnson, R. W. (1969) J. Petrology, 10, 409-439, (1574,1575).

_____, & Wilkinson, J. F. G. (1970) Contr. Mineral. and Petrology, 25, 241-269, (1576).

Nemoto, T. (1932) In: Leake, B. E. (1968) op. cit., (1577).

Nesbitt, R. W., & Hamilton, D. L. (1970) Phys. Earth Planet. Interiors, 3, 309-315, (2267-2270).

Nicholls, G. D. (1950) Q. Jl. geol. Soc. Lond., 106, 309-341, (2755-2759).

Nicholls, I. A. (1971) J. Petrology, 12, 67-119, (2711-2716).

Nicholls, J., & Carmichael, I. S. E. (1969) Contr. Mineral. and Petrology, 20, 268-294, (1578-1580).

Nickel, E. H., & Mark, E. (1965) Can. Mineral., 8, 105-197, (2266).

Nicolas, A., & Cagny, C. (1964) Geochemistry International, 1, 575-577, (2396).

Niggli, P. (1922) In: Leake, B. E. (1968) op. cit., (1581-1582).

Nikotina, L. P., Zeveleva, Ye Ye, & Marchak, V. P. (1967) Geochemistry International, 4, 783-789, (1583-1587).

Nockolds, S. R. (1935) Geol. Mag., 72, 289-317, (1588,1589).

_____, (1940) Q. Jl. Geol. Soc. Lond., 96, 451-510, (1590-1596).

_____, & Mitchell, R. L. (1948) Trans. Roy. Soc. Edinburgh, 61, 555-575, (2431-2437).

Morin, R. (1940) In: Leake, B. E. (1968) op. cit., (1597).

Novoselova, L. M. (1961) Ibid., (1598).

Novotny, M. (1949) Ibid., (1599-1605, 1612).

Ogura, Y. (1956) Ibid., (1606).

_____, (1958) Jap. J. Geol. Geogr., 29, 171-196, (1607-1610).

O'Hara, M. J. (1960) Geol. Mag., 97, 145-156, (1611).

_____, (1961) Mineral. Mag., 32, 848-865, (1613,1614).

_____, (1961) J. Petrology, 2, 248-276, (1615).

_____, & Mercy, E. L. P. (1963) Trans. Roy Soc. Edinburgh, 65, 251-314, (2419-2421).

Okamoto, Y. (1912) In: Leake, B. E. (1968) op. cit., (1616,1617).

Okrush, M. (1963) Ibid., (1618,1619).

Olsen, E. (1967) Science, 156, 61-62, (2708).

Ontoyev, D. O. (1958) In: Leake, B. E. (1968) op. cit., (1620).

Onuki, H. (1963) Ibid., (1621-1623).

_____, (1964) Ibid., (1624-1634).

_____, (1965) Ibid., (1635-1641).

_____, & Tiba, T. (1964) Ibid., (1642-1645).

_____, & Ernst, W. G. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 241-250, (2264,2265).

Orlov, A. (1932) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (2101).

Osann, A. (1891) In: Leake, B. E. (1968) op. cit., (1646).

_____ , (1913) Ibid., (1647).

_____, (1916) Ibid., (1647-1648).

Ovuinnikov, L. N. (1955) Ibid., (1650).

Pabst, A. (1928) Ibid., (1651).

Palache, C. (1894) In: Villiers, J. E. De (1948) Trans.

Geol. Soc. S. Africa, 51, 77-80, (2237).

_____, Davidson, S. C., & Coramson, E. A. (1930) Am. Miner., 15, 280-302, (1652).

Palache, E. (1935) In: Leake, B. E. (1968) op. cit., (1654).

Palmgren, J. (1917) Ibid., (1655).

_____, (1922) Ibid., (1656).

Palmunen, H. K. (1925) Ibid., (1657).

Pantin, H. M. (1956) Trans. Geol. Soc. Glasgow, 22, 48-78, (1658-1665).

Papike, J. J., & Clark, J. R. (1968) Am. Miner., 53, 1156-1173, (2500).

_____, Ross, M., & Clark, J. R. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 117-136, (2526-2530).

Parras, K. (1958) Bull. comm. geol. Finl., 181, (1666).

Parsons, A. L. (1930) Contr. Canadian Mineralogy, 29-33, (1667-1684).

Patterson, J. H., & O'Conner, D. J. (1966) Aust. J. Chem., 19, 1155-1164, (2422-2424).

Peacock, M. A. (1928) Am. Miner., 13, 241-286, (1681-1685).

Pecora, W. T., & Fischer, R. (1946) Ibid., 31, 370-385, (1686).

Pekun, I. F. (1951) In: Leake, B. E. (1968) op. cit., (1695,1696).

Peltola, E. (1960) Ibid., (1697).

Penfield, S. L., & Stanley, F. C. (1907) Am. J. Sci., 23, 23-51, (1698-1720).

Perchuk, L. L., Pavelenko, A. S., & Vernadskiy, V. I. (1967). Geochemistry International, 4, 850-869, (1730-1753).

Peters, T. (1963) Schweiz. miner. petrogr. Mitt., 43, 531-604, (1754).

Peters, Tj (1968) Contr. Mineral. and Petrology, 18, 65-75, (1755).

Phemister, R. (1950) Mineral. Mag., 29, 359-373, (54).

Phillips, W. J. (1956) Proc. Geol. Ass., 67, 103-121, (1757-1759).

Phillpotts, J. A., Schnetzler, C. C., & Thomas, H. H. (1972) Geochim. Cosmochim. Acta, 36, 1131-1166, (2764-2766).

Pirani, R. (1951) In: Leake, B. E. (1968) op. cit., (1760,1761).

———, (1952) Ibid., (1766).

———, (1953) Ibid., (1767).

Pisani, F. (1877) In: Rabbit , J. C. (1948) Am. Miner., 33, 264-323, (1815,1816).

———, In: Evans, H. M., & Bancroft, J. A. (1908) Am. J. Sci., 26, 509-512, (637).

Polovinkina, Y. I. (1924) In: Leake, B. E. (1968) op. cit., (1762).

Polovoko, N. I., Siroshtan, R. I., & Riabokan, S. K. (1960) Ibid., (1763-1765).

Poubova, L. (1971) Krystalinikum, 7, 119-133, (2791-2799).

Prakash, D., & Dalela, I. K. (1964) Am. Miner., 49, 424-427, (1768,1769).

Pratt, J. H. (1898) In: Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1803).

Prewitt, C. T. (1963) Geol. Soc. Amer. Spec. Paper, 73, 132-133, (2802,2803).

Prider, R. T. (1939) Mineral. Mag., 25, 373-387, (1770).

Prinz, M., & Nehru, C. E. (1969) Ibid., 37, 372-337, (2720-2727).

Quensel, P. (1914) In: Billings, M. (1928) Am. Miner., 13, 287-296, (179).

Rabbit , J. C. (1948) Am. Miner., 33, 263-323, (1773-1779).

Rajagopalan, C. (1946) In: Leake, B. E. (1968) op. cit., (1780).

Rajesekaran, K. C. (1961) Ibid., (1781).

Rama, B. Rao, (1937) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (1801).

Ramachandra, M. B. Rao, (1937) In: Leake, B. E. (1968) op. cit., (1782,1783).

Ramberg, H. (1943) Ibid., (1784-1786).

Rammelsberg, C. F. (1850) Ibid., (1278).

_____, In: Harrington, B. J. (1903) Am. J. Sci., 15, 392-394, (798).

Ravier, J. (1951) In: Leake, B. E. (1968) op. cit., (1788).

Raychaudhuri, B. (1960) Ibid., (1789-1794).

_____, (1964) Am. Miner., 49, 198-206, (1795-1800).

Read, H. H. (1934) Mineral. Mag., 23, 519-540, (1823).

Reed, J. J. (1958) In: Leake, B. E. (1968) op. cit., (1824,1825).

Reinecke, L., & McClure, L. (1939) Trans, Geol. Soc. S. Africa, 36, 32, (780-785).

Renard, A. & Klement, C. (1884) In: Peacock, M. A. (1928) Am. Miner., 13, 241-286, (1660).

Rhein, C. H. (1967) In: Leake, B. E. (1968) op. cit., (1826).

Richarz, S. (1930) Am. Miner., 15, 65-68, (1827).

Ridley, I. (1971) Contr. Mineral. and Petrology, 32, 251-266, (1828).

Rimman, E. (1936) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323,

Robinson, P., & Jaffe, H. W. (1969) Mineral. Soc. Amer. Spec. Paper, 2, 251-274, (2541-2551).

_____, _____, (1969) Am. J. Sci., 267, 389-421, (2531-2534).

_____, _____, Klein, C. Jr., & Ross, M. (1969) Contr. Mineral. and Petrology, 22, 249-258, (2535-2540).

_____, _____, Ross, M., & Klein, C. Jr. (1971) Am. Miner., 56, 909-939, (1829,1830).

Rodolico, F. (1931) In: Leake, B. E. (1968) op. cit., (1831).

Rondolino, R. (1936) Ibid., (1832-1834).

Roonwall, G. S. (1972) Geol. Rdsch., 61, 282-301, (2665-2667).

Rose, G. (1842) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (1618).

Rose, H., & Fromme, J. (1932) In: Leake, B. E. (1968) op. cit.,

(1935).

Rosenbusch, H. (1910) Ibid., (608,1036).

Rosenzweig, A., & Watson, E. E. (1954) Am. Miner., 39, 581-599, (1037-1044).

Rosicky, V. (1902) In; Rabbit, J. C. (1948) Am. Miner., 33, 273-323, (1004).

Ross, C. S. (1929) Econ. Geol., 24, 641-645, (1045).

_____, (1941) In: Leake, B. E. (1968) op. cit., (1046,1047).

Ross, M., Papike, J. J., & Shaw, K. W. (1969) Mineral. Soc. Amer. Spec. Paper., 2, 275-299, (2554).

_____, _____, & Weiblen, P. W. (1968) Science, 159,(1099-1102,2552-2553).

Roumhet, P. G., Gillard, J. L., & Fripiat, J. J. (1972) Mineral. Mag., 38, 583-592, (2704,2705).

Roy, S. (1970) Ibid., 37, 708-716, (2728-2736).

Rucklidge, J. C., Gasparrini, E., Smith, J. V., & Knowles, C. R. (1971) Can. J. Earth Sci., 8, 1171-1183, (1049-1065).

Ruckmick, J. C., & Noble, J. A. (1959) Bull. Geol. Soc. Amer., 70, 981-1018, (1067).

Sabine, P. A. (1910) Geol. Surv. Gt. Britain Bull., 16, 156-177, (1068).

Sadashivaiah, M. S. (1962) In: Leake, B. E. (1968) op, cit., (1069).

Sahama, T. G. (1947) Bull. commn. geol. Finl., 140, 159-162, (290,1970).

_____, (1956) Am. Miner., 41, 509-512, (1971).

Sahlstein, T. G. (1935) Meddel. om Gronland, 95, (1972).

Saksela, M. (1960) In: Leake, B. E. (1968) op. cit., (1973).

Sakurai, K., Ashizawa, T. (1955) Ibid., (1974).

Salotti, C. A. (1962) Am. Miner., 47, 1055-1066, (1975).

Sameshima, T. (1949) In: Leake, B. E. (1968) op. cit., (1976-1978).

Sarap. H. (1957) Ibid., (1979).

Saravanan, S., & Ramasamy, P. (1971) Mineral. Mag., 38, 376-377, (2765).

Sateo, H. (1930) In: Leake, B. E. (1968) op. cit., (1980).

Savolahti, A. (1962) Bull. comm. geol. Finl., 204, 33-112, (1981).

_____, (1966) Ibid., 222, 173-197, (2839).

Schalder, J. (1914) In: Moritsch, et. al. (1960) Tschermaks miner. petrogr. Mitt., 7, 210-217, (842).

Schirmeisen, C. F. (1914) In: Rabbit, J. C. (1948) Am. Miner. 33, 263-323, (2006).

Schneider, C. (1891) In: Leake, B. E. (1968) op. cit., (1982-1989).

Schubert, W. (1969) Contr. Mineral. and Petrology, 21, 295-310, (1990-1993).

Schurmann, H. M. E. (1938) In: Leake, B. E. (1968) op. cit., (1994).

Schwander, H. (1960) Ibid., (1995).

Scott, A. (1914) Mineral. Mag., 17, 138-142, (1997).

Segeler, C. G. (1961) Am. Miner., 46, 637-641, (1998-2001).

Seitsaari, J. (1951) Bull. comm. geol. Finl., 153, (2002,2003).

_____, (1952) Ann. Acad. Sci. Fennicae, 30, (2837,2838).

_____, (1953) Ibid., 159, 83, (2004-2006).

_____, (1956) Ibid., 172, 77-83, (2007).

Seki, Y. (1958) Jap. J. Geol. Geogr., 29, 231-258, (2008-2011).

_____, Aiba, M., & Kato, C. (1959) Ibid., 30, 233-243, (2012-2016).

_____, & Kuriyagowa, S. (1962) Ibid., 33, 15-22, (2017).

_____, Yamasaki, M. (1957) Am. Miner., 42, 506-520, (2018).

Sen, N., Nockolds, S. R., & Allen, R. (1959) Geochim. Cosmochim. Acta, 16, 58-78, (2019-2023).

Serdiuchenko, D. P. (1938) In: Leake, B. E. (1968) op. cit., (2024-2026).

———————, (1954) Ibid., (2027-2029).

———————, (1959) Ibid., (2030).

———————, (1968) Mineral. Soc. I.M.A. vol. (I.M.A. papers and proc. 5th gen. meeting, Cambridge 1966), 285-290, (2436-2447).

Shannon, E. V. (1924) In: Billings, L. (1928) Am. Miner., 13, 287-296, (181).

Sharma, T. (1967) Bull. Geochem. Soc. India, 2, 15-19, (2262, 2263).

Shevenko, E. V. (1959) In: Leake, B. E. (1968) op. cit., (2037-2039).

Shibata, K. (1944) Ibid., (2040, 2041).

Shido, F. (1958) J. Geol. Soc. Japan, 64, 595, (160).

———————, (1958) J. Fac. Sci. Tokyo Univ., 11, 131-218, (2047-2050).

———————, (1959) In: Leake, B. E. (1968) op. cit., (2042-2046).

———————, (1959) Ibid., (2000).

———————, & Miyashiro, A. (1959) J. Fac. Sci. Univ. Tokyo, 12, 85-102, (2059-2067).

———————, & Seki, Y. (1959) J. Geol. Soc. Japan, 65, 673-677, (2801).

Shimozu, K. (1963) In: Leake, B. E. (1968) op. cit., (2068-2070).

Shynukov, E. F. (1958) Ibid., (2071).

Simonen, A. (1948) Bull. comm. geol. Finl., 143, 1-66, (2072-2074).

———————, (1960) Ibid., 189, (2075-2076).

Simpson, E. S. (1933) In: Leake, B. E. (1968) op. cit., (2077).

———————, (1936) Ibid., (2078).

Siroshtan, R. I., & Polovoko, K. I. (1959) Ibid., (2079-2083).

Sjorgren, H. (1882) In: Rabbit, J. C. (1948) Am. Miner., 33. 263-323, (2090).

Slavik, F., & Vesely, V. (1927), Ibid., (2104).

Smith, & Brush (1853) Am. J. Sci., 14, 369, (2300, 2301).

Smith, W. C., Hey, M. H., & Kempe, D. R. C. (1968) Mineral.

Mag., 36, 1164-1167, (2084).

Snelling, N. C. (1958) In: Leake, B. E. (1968) op. cit., (2086).

_____, (1960) Q. Jl. Geol. Soc. Lond., 116, 187-213. (2087).

Sobolev, N. D. (1959) In: Leake, B. E. (1968) op. cit., (2088).

Sobolev, V. (1947) Ibid., (2089).

Somasekar, B., & Sadashivaiah, M. S. (1961) Ibid., (2125).

Stappenbeck, R. (1932) In; Rabbit J. C. (1948) Am. Miner. , 33, 263-323, (1907).

Starreba, F. S. (1947) In: Leake, B. E. (1968) op. cit., (2121).

Steenstrup, K. J. V. (1877) In: Boggild, O.B. (1905) Meddel. om Gronland, 32, (201).

Steiger, R. (1961) Schweiz. miner. petrogr. Mitt., 41, 127-156, (2106-2120).

Stout, J. H. (1971) Am. Miner., 56, 212-224, (2122-2127).

_____, (1972) J. Petrology, 13, 99-145, (2607-2660).

Strand, T. (1951) In: Leake, B. E.(1968) op. cit., (2128-2130).

Strecheisen, A. (1954) Schweiz. miner. petrogr. Mitt., 34; 336-409, (2131-2132).

Subbarao, K. V. (1965) In: Leake, B. E. (1968) op. cit., (2133, 2134).

_____, (1971) J. Petrology, 12, 621-641, (2739,2740).

Subramaniam, A. P. (1956) Bull. Geol. Soc. Amer., 67, 317-390, (2135-2138).

Sugi, K. (1931) In: Leake, B. E. (1968) op. cit., (2139).

_____, (1935) Ibid., (2140-2143).

Sunagawa, I. (1952) Ibid., (2144).

Sundius, N. (1924) Ibid., (2145).

_____, (1931) Am. J. Sci., 21, 330-344, (2146-2149).

_____, (1945) In: Bilgrami, G. A. (1955) Mineral. Mag., 30, 633-644, (172).

_____, (1946) Ibid., (174).

Geochemistry International, 7, 140-151, (2352).

Yoshimura, T. (1939) In: Leake, B. E. (1968) op. cit., (2353,2354).

_____, (1940) Ibid., (2355).

Yoshizawa, K. (1941) In: Brown, F. E. (1956) Geol. Lab., 93, 72-84, (291).

Zambonini, F. (1902) In: Bearth, P. (1959) Schweiz. miner. petrogr. Mitt., 39, 267-286, (144).

Zambonini, F. (1905) In: Leake, B. E. (1968) op. cit., (2356).

Zartman, R. E. (1964) J. Petrology, 5, 359-408, (2357).

Zussman, J. (1955) Acta Crystallogr., 8, 301-308, (2494).

_____, (1959) Ibid., 12, 309-312, (2495).

———————, (1946) Sver. Geol. Under., 40, (2152-2154, 2210-2211).

Sustschinsky, M. (1912) In: Eskola, P. (1914) Bull. commn. Geol. Finl., 44, (617).

Sutherland, D. S. (1967) Contr. Mineral. and Petrology, 24, 114-135, (2155-2160).

Switzer, G. (1951) In: Ernst, W. G., & Wai, C. M. (1970) Am. Miner., 55, 1226-1259, (606).

Tajder, M. (1939) In: Leake, B. E. (1968) op. cit., (2161).

Takubo, J., & Ukai, Y. (1954) Jap. J. Geol. Geogr., 24, 145-159, (2162-2166).

Taneda, S. (1947) Mem. Fac. Sci. Kyusyu Univ., 3, 13, (2167).

Tanner, P. W. G., & Tabisch, O. T. (1972) Scott. J. Geol., 8, 151-178, (2582).

Teall, J. E. (1888) Mineral. Mag., 8, 116-120, (2168-2169).

Thomson, T. (1836) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (2097).

Tiba, T., Hashimoto, H., & Kato, A. (1970) Lithos, 3, 335-340, (2170,2171).

Tikhonenkova, R. P. (1959) In: Leake, B. E. (1968) op. cit., (2172,2173).

Tilley, C. E. (1938) Geol. Mag., 75, 497-511, (2174-2176).

———————, (1939) Ibid., 76, 326-330, (2177).

———————, (1957) Am. Miner., 42, 412-416, (2178-2179).

———————, & Flett, J. S. (1930) Summ. Progress Geol. Surv. Gt. Britain, for 1929, Pt. 2, 24-40, (2180,2181).

Toit, A. L. du, (1945) Trans, Geol. Soc. S. Africa, 48, 161-206, (2182,2183).

Tomita, I. (1962) In: Leake, B. E. (1968) op. cit., (2184-2190).

Toulmin, P. (1964) Ibid., (2191-2192).

Trenzen, C. (1902) Ibid., (2193).

Trojer, F., & Walitzi, E. L. (1965) Tschermaks miner. petrogr. Mitt., 10, 237-240, (2194).

Troll, G., & Gilbert, M. C. (1972) Am. Miner., 57, 1386-1403, (2587).

Trommsdorff, V., & Evans, B. W. (1972) Am. J. Sci., 272, 423-437, (2698-2703).

Tsuboi, S. (1935) In: Leake, B. E. (1968) op. cit., (2195).

_____, (1936) In: Banno, S. (1964) J. Fac. Sci. Tokyo Univ., 15, 203-319, (104).

_____, (1938) In: Leake, B. E. (1968) op. cit., (2196).

Uchimuzu, K. (1966) J. Fac. Sci. Tokyo Univ., 16, 85-159, (2197).

Ueda, T., & Tomita, K. (1963) Mineral. J. Japan, 4, 85-90, (2261).

Ui, T. (1971) J. Fac. Sci. Tokyo Univ., 18, 53-127, (2364-2366).

Uralsky, B. F., & Buchneva, S. K. (1939) In; Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (1805,1806).

Ussing, N. V. (1890) In: Eskola, P. (1914) Bull. comm. geol. Finl., 40, (912).

Vahatalo, V. O. (1953) Bull. comm. geol. Finl., 164, (2198).

Valiquette, G., & Archambault, G. (1970) Can. Mineral., 10, 485-510, (2200,2201).

Van der Plas, L. (1959) In: Leake, B. E. (1968) op. cit., (2202).

_____, & Hugi, Th, (1961) Schweiz. miner. petrogr. Mitt., 41, 371-393, (2203).

Van Horn, F. R. (1897) In: Leake, B. E. (1968) op. cit., (2204).

Vande Putte, R. (1939) Ibid., (2205-2222).

Varne, R. (1968) J. Petrology, 9, 169-190, (2223,2224).

Velde, B., Herve, F., & Kornprobst, J. (1970) Am. Miner., 55, 953-974, (2226-2228).

Velde, D. (1971) Contr. Mineral. and Petrology, 30, 216-239, (2225).

Vendle, B. (1924) In: Eskola, P. & Sahlstein, A.L. (1930)

Bull. comm. geol. Finl., 92, 77-95, (625).

Vendle, L. (1924) Mineral. Mag., 22, 237-240, (2229).

Venugopal, J. S., & Sadashivaiah, M. S. (1960) In: Leake, B. E. (1968) op. cit., (2230).

Vermaas, F. H. S. (1952) Trans. Geol. Soc. S. Africa, 55, 199-229, (2231-2235).

Vernon, R. H. (1962) Am. Miner., 47, 360-370, (2234,2235).

Villiers, J. E. de (1940) Trans. Geol. Soc. S. Africa, 51, 77-80, (2236).

Vincent, E. A. (1953) Q. Jl. geol. Soc. Lond., 109, 21-49, (2238).

Vinogradskaya, G. M. (1959) In; Leake, B. E. (1968) op. cit., (2239).

Vlasov, K. A., Kuzmenko, M. V., & Eskova, E. M. (1966) The Lovozerro Alkali Massif, Oliver & Boyd, 627pp. (2257-2260).

Volkov, V. P., Polykov, A. I.& Marakhanova, M. I. (1962) Geochemistry Ann. Arbor., 561-570, (2240-2242).

Wade, A., & Prider, R. T. (1940) Q. Jl. geol. Soc. Lond., 96, 39-97, (2243).

Wahlstrom, E. E. (1934) Am. Miner., 19, 178-180, (2244).

———————, (1940) Econ. Geol., 35, 477-500, (2245).

Walker, T. L. (1924) Univ. Toronto Studies. Geol. ser., 58-61, (2390,2391).

———————, & Parsons, A. L. (1927) Contr. Canadian Mineralogy (Toronto), 15-30, (2389).

Walker, T. R., Ribbe, P. H., & Honea, R. M. (1967) Bull. Geol. Soc. America, 78, 1055-1060, (2246-2248).

Warren, H. V. (1951) Mineral. Mag., 22, 477-481, (2249,2250).

Washington, H. S. (1914) Am. J. Sci., 38, 79-90, (2255).

———————, (1922) In: Leake, B. E. (1968) op. cit., (2256).

———————, & Merwin, H. E. (1922) Am. Miner., 7, 121-125, (2273).

———————, ———————, (1923) Ibid., 8, 63-67, (2274).

———————, & Wright, F. E. (1908) Am. J. Sci., 26, 187-211, (2252,2253).

Watanbe, J. (1965) In: Leake, B. E. (1968) op. cit., (2275-2291).

Watanbe, N., & Yagi, K. (1953) Ibid., (2292).

Weeks, W. F. (1956) J. Geol., 64, 456-472, (2293-2295).

Weibel, M., & Locher, T. (1964) Schweiz. miner. petrogr. Mitt., 44, 158-185, (2296).

Weibull, M. (1896) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (2102).

Weidman, S. (1903) Am. J. Sci., 15, 227-232, (2297).

———————, (1907) In: Leake, B. E. (1968) op. cit., (2302).

Weyberg, Z. (1912) Ibid., (2304,2305).

White, A. J. R., Chappell, B. W., & Jakes, P. (1972) Contr. Mineral. and Petrology, 34, 185-191, (2305).

Whittaker, E. J. W. (1949) Acta Crystallogr., 2, 312-317, (2496).

———————, (1969) Ibid., B25, 394-397, (2497).

Weisander, H. (1932) In: Rabbit, J. C. (1948) Am. Miner., 33, 263-323, (2103).

Wiik, F. J. (1878) Ibid., (2091,2092).

———————, (1880) In: Eskola, P. (1914) Bull. commn. geol. Finl., 40, 274, (614,615).

Wikstrom, A. (1970) Norsk. geol. tiddskr., 50, 137-155, (2307-2314).

Wilcox, R. E., & Poldervaart, A. (1958) Bull. Geol. Soc. Amer., 69, 1323-1368, (2315).

Wilkins, R. W. T., Davidson, L. R., & Ross, J. R. (1970) Contr. Mineral. and Petrology, 28, 280-287, (2498,2499).

Wilkinson, J. F. G. (1961) Am. Miner., 46, 340-354, (2316).

———————, (1963) J. Petrology, 3, 192-214, (2317).

———————, (1971) Ibid., 12, 587-619, (2706,2707).

———————, Vernon, R. H., & Shaw, S. E. (1964) Ibid., 5, 461-488, (2318,2319).

Willbourn, F. S. (1926) Mining Mag., 35, 329-338, (2320).

Williams, A. F. In: Hall, A. (1930) Geol. Surv. S. Africa, 32, (702).

Williams, G. H. (1886) In: Hertz, H. (1951) Bull. Geol. Soc. Amer., 52, 978-1016, (869).

Wilshire, H. G., & Trask, N. J. (1971) Am. Miner., 56, 240-255, (2321).

Winchell, A. N. (1931) Ibid., 16, 250-266, (2324-2329).

Winchell, H. In: Leake, B. E. (1968) op. cit., (2332).

Wise, W. (1969) Bull. Geol. Soc. Amer., 80, 969-1006, (2336,2337).

Wise, W. S. (1966) Bull. Volcan., 29, 235-252, (2761).

Wiseman, J. D. H. (1934) Q. Jl. geol. Soc. Lond., 90, 354-415, (2338-2340).

Wittels, M. (1952) Am. Miner., 37, 28-36, (2741).

Wolff, J. E. (1929) J. Geol., 37, 1-16, (2342).

———————, (1937) Am. Miner., 22, 742-744, (2343).

———————, (1938) Bull. Geol. Soc. Amer., 49, 1569-1626, (2344).

Wolff, T. F. von (1942) In: Leake, B. E. (1968) op. cit., (2345).

Wolley, A.R., Symes, R. F., & Elliott, C. J. (1972) Mineral. Mag., 38, 819-836, (2563-2579).

Wright, F. E. (1900) In: Billings, M. (1928) Am. Miner., 13, 287-296, (186).

Yagi, K. (1953) Bull. Geol. Soc. Amer., 64, 769, (34,48,176).

Yakoleva, A. K., & Kolesnikova, V. V. (1967) In: Misch, H. J. (1969) Contr. Mineral. and Petrology., 21, 319-331, (1047,1048).

Yakoleva, K. E. (1961) In: Leake, B. E. (1968) op. cit., (2346, 2347).

Yen, T. P. (1959) Ibid., (2348-2351).

Yershova, Z. P., Babeshin, A. M., & Perifil'yev, Yu, D. (1970)

Table A8.2. The two numerically largest oxide weight per cent values in each of the chemical analyses in the amphibole data file.

1	SIO2	39.64	FEO	25.15	41	SIO2	38.30	AL2O3	12.87
2	SIO2	42.17	MGO	14.46	42	SIO2	38.24	AL2O3	15.48
3	SIO2	43.22	FEO	17.31	43	SIO2	38.44	AL2O3	15.87
4	SIO2	46.68	AL2O3	14.37	44	SIO2	42.52	AL2O3	11.25
5	SIO2	58.59	MGO	24.78	45	SIO2	39.68	AL2O3	14.48
6	SIO2	57.35	MGO	23.87	46	SIO2	38.78	AL2O3	14.67
7	SIO2	56.92	MGO	23.81	47	SIO2	43.06	MGO	14.90
8	SIO2	56.36	MGO	22.97	48	SIO2	48.51	FE2O3	17.53
9	SIO2	58.24	MGO	25.16	49	SIO2	47.54	FEO	23.21
10	SIO2	34.18	FEO	21.98	50	SIO2	48.41	FEO	23.81
11	SIO2	37.78	FEO	24.46	51	SIO2	50.79	FEO	20.56
12	SIO2	47.01	MGO	12.78	52	SIO2	52.41	FEO	14.82
13	SIO2	58.72	MGO	13.25	53	SIO2	50.25	FEO	17.09
14	SIO2	54.41	MGO	24.86	54	SIO2	51.30	FEO	18.50
15	SIO2	52.30	MGO	28.10	55	SIO2	40.70	MGO	14.74
16	SIO2	55.56	MGO	21.97	56	SIO2	38.76	AL2O3	15.42
17	SIO2	57.34	MGO	24.77	57	SIO2	39.99	AL2O3	15.03
18	SIO2	52.50	MGO	17.00	58	SIO2	38.04	AL2O3	15.21
19	SIO2	53.20	MGO	19.10	59	SIO2	39.21	AL2O3	15.01
20	SIO2	57.30	MGO	20.90	60	SIO2	39.89	AL2O3	15.08
21	SIO2	52.30	MGO	17.60	61	SIO2	39.26	AL2O3	15.15
22	SIO2	42.50	FEO	20.70	62	SIO2	41.55	AL2O3	14.15
23	SIO2	39.30	FEO	27.90	63	SIO2	40.53	AL2O3	14.68
24	SIO2	39.30	FEO	29.90	64	SIO2	41.05	AL2O3	14.50
25	SIO2	52.20	MGO	17.60	65	SIO2	40.63	AL2O3	14.49
26	SIO2	53.00	MGO	17.60	66	SIO2	41.59	MGO	15.42
27	SIO2	56.20	MGO	22.60	67	SIO2	42.49	MGO	14.57
28	SIO2	57.30	MGO	25.00	68	SIO2	42.06	AL2O3	14.58
29	SIO2	52.80	MGO	19.10	69	SIO2	41.40	AL2O3	13.43
30	SIO2	51.50	MGO	17.00	70	SIO2	41.42	MGO	12.12
31	SIO2	54.60	MGO	22.30	71	SIO2	41.96	MGO	13.40
32	SIO2	44.50	FEO	19.80	72	SIO2	41.84	MGO	14.27
33	SIO2	41.14	MGO	14.08	73	SIO2	42.40	MGO	15.53
34	SIO2	40.73	FEO	11.91	74	SIO2	39.47	AL2O3	15.30
35	SIO2	40.27	FEO	12.45	75	SIO2	38.90	FEO	15.20
36	SIO2	39.68	AL2O3	12.81	76	SIO2	39.05	AL2O3	15.74
37	SIO2	38.90	AL2O3	16.02	77	SIO2	38.90	AL2O3	14.70
38	SIO2	39.68	AL2O3	14.82	78	SIO2	38.64	AL2O3	16.22
39	SIO2	39.20	AL2O3	13.87	79	SIO2	38.16	FEO	15.81
40	SIO2	39.26	AL2O3	13.42	80	SIO2	37.74	AL2O3	17.71

81	SIO2	37.70	FEO	17.49
82	SIO2	37.30	FEO	18.03
83	SIO2	37.20	FEO	19.97
84	SIO2	36.69	AL2O3	19.90
85	SIO2	36.53	FEO	21.39
86	SIO2	36.45	FEO	21.91
87	SIO2	36.35	FEO	20.19
88	SIO2	33.50	AL2O3	17.89
89	SIO2	43.14	FEO	14.41
90	SIO2	48.83	FEO	21.77
91	SIO2	49.83	FEO	18.86
92	SIO2	35.65	FEO	12.04
93	SIO2	49.49	MGO	13.97
95	SIO2	48.13	FEO	11.82
96	SIO2	50.35	MGO	13.00
97	SIO2	47.97	FEO	11.75
98	SIO2	48.29	MGO	13.19
99	SIO2	46.16	FEO	13.70
100	SIO2	41.10	AL2O3	13.75
101	SIO2	44.47	AL2O3	13.11
102	SIO2	43.07	AL2O3	15.04
103	SIO2	44.92	MGO	13.59
104	SIO2	47.85	MGO	13.19
105	SIO2	46.06	MGO	14.78
106	SIO2	48.84	MGO	17.29
107	SIO2	48.25	MGO	12.12
108	SIO2	43.55	AL2O3	12.09
109	SIO2	52.03	MGO	14.23
110	SIO2	43.99	AL2O3	16.06
111	SIO2	40.85	FEO	14.12
112	SIO2	48.40	MGO	16.20
113	SIO2	48.35	CAO	12.52
114	SIO2	46.65	CAO	11.95
115	SIO2	45.20	MGO	13.47
116	SIO2	47.05	CAO	10.87
117	SIO2	47.30	CAO	10.87
118	SIO2	44.95	FEO	15.80
119	SIO2	46.50	CAO	12.37
120	SIO2	45.18	MGO	12.12
121	SIO2	44.30	CAO	13.21
122	SIO2	45.26	FE2O3	11.07
123	SIO2	43.00	AL2O3	13.30
124	SIO2	45.75	CAO	12.21
125	SIO2	45.26	MGO	15.40
126	SIO2	45.18	MGO	14.00
127	SIO2	42.50	FEO	14.10
128	SIO2	44.20	MGO	12.05
129	SIO2	43.88	MGO	11.66
130	SIO2	45.55	FEO	12.80
131	SIO2	40.50	FEO	12.95
132	SIO2	43.59	MGO	14.59
133	SIO2	43.59	MGO	14.59
134	SIO2	41.02	FEO	16.51
135	SIO2	41.02	FE2O3	23.40
136	SIO2	44.40	FEO	15.70
137	SIO2	44.40	FEO	20.00
138	SIO2	45.20	FEO	12.50
139	SIO2	35.17	AL2O3	15.83
140	SIO2	41.81	AL2O3	15.15
141	SIO2	37.72	FEO	23.42
142	SIO2	57.50	AL2O3	12.50
143	SIO2	57.81	MGO	13.07
144	SIO2	55.43	AL2O3	12.26
145	SIO2	57.73	MGO	13.02
146	SIO2	37.01	FEO	22.15
147	SIO2	43.62	FEO	13.06
148	SIO2	52.87	MGO	20.14
149	SIO2	49.89	MGO	16.51
150	SIO2	47.82	MGO	14.61
151	SIO2	46.80	MGO	14.57
152	SIO2	42.92	FEO	12.74
153	SIO2	42.60	FEO	12.87
154	SIO2	40.96	AL2O3	15.35
155	SIO2	40.58	MGO	13.82
156	SIO2	40.47	AL2O3	15.66
157	SIO2	40.64	MGO	14.75
158	SIO2	40.29	AL2O3	16.54
159	SIO2	40.00	AL2O3	14.63
160	SIO2	40.00	AL2O3	14.83
161	SIO2	40.64	AL2O3	14.07

162	SIO2	40.32	AL2O3	14.00
163	SIO2	39.79	AL2O3	14.26
164	SIO2	46.70	MGO	13.35
165	SIO2	40.66	FEO	17.72
166	SIO2	55.14	MGO	22.16
167	SIO2	55.64	MGO	22.09
168	SIO2	53.73	MGO	20.60
169	SIO2	53.26	MGO	29.16
170	SIO2	53.26	MGO	29.16
171	SIO2	53.25	MGO	28.42
172	SIO2	57.74	MGO	23.67
173	SIO2	51.21	MGO	11.31
174	SIO2	57.10	MGO	9.13
175	SIO2	52.66	FE2O3	18.44
176	SIO2	48.51	FE2O3	17.53
177	SIO2	46.61	AL2O3	12.04
178	SIO2	42.28	MGO	14.38
179	SIO2	37.49	FEO	25.14
180	SIO2	37.40	FEO	25.84
181	SIO2	38.50	FEO	27.28
182	SIO2	38.04	FEO	15.85
183	SIO2	38.63	CAO	12.81
184	SIO2	39.23	AL2O3	14.38
185	SIO2	43.30	MGO	16.02
188	SIO2	44.18	FEO	13.90
189	SIO2	49.80	FEO	40.10
190	SIO2	49.68	MGO	13.39
191	SIO2	44.60	MGO	15.40
192	SIO2	40.14	AL2O3	14.50
193	SIO2	53.40	FEO	16.23
194	SIO2	53.80	FEO	17.88
195	SIO2	55.20	FEO	12.40
196	SIO2	50.20	FEO	30.40
197	SIO2	55.56	MGO	19.45
198	SIO2	45.07	MGO	14.97
199	SIO2	40.26	AL2O3	13.09
200	SIO2	50.37	MGO	19.75
201	SIO2	46.18	MGO	25.05
202	SIO2	44.24	FEO	29.46
203	SIO2	55.82	MGO	20.61
204	SIO2	57.49	MGO	12.95
205	SIO2	57.93	AL2O3	11.92
206	SIO2	56.72	MGO	10.56
207	SIO2	56.38	MGO	9.89
208	SIO2	55.38	FEO	13.07
209	SIO2	55.10	FE2O3	10.61
210	SIO2	51.17	FEO	18.48
211	SIO2	49.87	FEO	20.19
212	SIO2	48.30	FEO	20.40
213	SIO2	40.21	AL2O3	14.80
214	SIO2	40.20	MGO	14.61
215	SIO2	41.35	MGO	14.92
216	SIO2	40.73	MGO	15.68
217	SIO2	41.25	MGO	15.90
218	SIO2	42.23	MGO	16.40
219	SIO2	53.19	MGO	20.57
220	SIO2	57.21	MGO	30.51
221	SIO2	50.25	FEO	17.09
222	SIO2	48.09	FEO	25.33
223	SIO2	47.45	FEO	21.41
224	SIO2	47.70	FEO	22.57
225	SIO2	47.60	FEO	22.35
226	SIO2	48.59	FEO	21.10
227	SIO2	49.60	FEO	22.24
228	SIO2	48.44	FEO	21.12
229	SIO2	48.74	FEO	21.52
230	SIO2	49.15	FEO	20.60
231	SIO2	48.47	FEO	22.93
232	SIO2	49.61	FEO	19.50
233	SIO2	50.19	FEO	20.53
234	SIO2	47.56	FEO	26.03
235	SIO2	40.20	FEO	25.52
236	SIO2	39.43	FEO	25.59
237	SIO2	38.08	FEO	28.81
238	SIO2	38.10	FEO	27.50
239	SIO2	41.70	FEO	28.32
240	SIO2	39.10	FEO	26.61
241	SIO2	40.98	FEO	22.31
242	SIO2	39.32	FEO	21.93
243	SIO2	46.57	FEO	31.38

244	SIO2	37.34	FEO	20.40
245	SIO2	36.73	FEO	21.43
246	SIO2	36.80	FEO	23.74
247	SIO2	37.08	FEO	22.02
248	SIO2	37.48	FEO	19.16
249	SIO2	37.50	FEO	14.20
250	SIO2	39.00	AL2O3	13.50
251	SIO2	36.60	FEO	16.50
252	SIO2	35.90	FEO	17.80
253	SIO2	37.80	AL2O3	13.60
254	SIO2	38.30	FEO	20.00
255	SIO2	37.90	AL2O3	13.00
256	SIO2	36.80	FEO	21.20
257	SIO2	37.80	AL2O3	13.40
258	SIO2	37.90	AL2O3	13.40
259	SIO2	38.10	FEO	17.90
260	SIO2	38.70	FEO	19.00
261	SIO2	36.60	FEO	22.10
262	SIO2	39.60	MGO	13.80
263	SIO2	38.50	AL2O3	13.60
264	SIO2	38.50	FEO	14.50
265	SIO2	40.60	FEO	12.90
266	SIO2	39.00	MGO	13.30
267	SIO2	42.30	MGO	13.80
268	SIO2	41.00	MGO	12.50
269	SIO2	41.48	FEO	14.93
270	SIO2	36.95	FEO	19.40
271	SIO2	38.84	FEO	24.14
272	SIO2	47.40	MGO	14.61
273	SIO2	47.09	CAO	13.51
274	SIO2	44.34	MGO	13.08
275	SIO2	43.97	AL2O3	14.50
276	SIO2	42.70	FEO	13.78
277	SIO2	42.09	MGO	16.16
278	SIO2	41.20	FEO	12.43
279	SIO2	42.92	FEO	11.98
280	SIO2	38.56	FEO	18.72
281	SIO2	37.13	FEO	21.55
282	SIO2	40.29	CAO	11.83
283	SIO2	45.98	MGO	17.92
284	SIO2	52.00	FEO	18.00
285	SIO2	53.30	MGO	14.80
286	SIO2	53.30	FEO	17.10
287	SIO2	52.00	FEO	16.40
288	SIO2	54.30	FEO	15.00
289	SIO2	38.77	FEO	26.54
290	SIO2	38.24	FEO	26.64
291	SIO2	37.88	FEO	26.08
292	SIO2	53.56	MGO	19.85
293	SIO2	51.33	MGO	19.49
294	SIO2	56.14	MGO	22.02
295	SIO2	53.99	MGO	20.59
296	SIO2	56.80	MGO	21.97
297	SIO2	56.32	MGO	21.85
298	SIO2	58.34	MGO	24.90
299	SIO2	46.70	MGO	12.60
300	SIO2	42.30	AL2O3	16.30
301	SIO2	51.90	MGO	20.50
302	SIO2	53.60	MGO	18.80
303	SIO2	42.66	FEO	14.18
304	SIO2	43.13	AL2O3	13.09
305	SIO2	42.03	AL2O3	12.59
306	SIO2	42.91	AL2O3	12.45
307	SIO2	42.66	MGO	13.15
308	SIO2	43.60	MGO	12.41
309	SIO2	41.25	FEO	13.50
310	SIO2	41.06	AL2O3	15.47
311	SIO2	40.54	AL2O3	14.43
312	SIO2	39.78	FEO	14.21
313	SIO2	39.32	FEO	20.43
314	SIO2	37.90	FEO	20.71
315	SIO2	38.44	FEO	24.67
316	SIO2	41.25	FEO	16.28
317	SIO2	38.73	FEO	22.89
318	SIO2	38.74	FEO	23.28
319	SIO2	42.50	AL2O3	15.65
320	SIO2	51.67	MGO	23.37
321	SIO2	41.38	AL2O3	14.41
322	SIO2	46.79	MGO	20.17
323	SIO2	47.08	FEO	35.65

324	SIO2	45.50	MGO	20.00
325	SIO2	42.30	FEO	12.10
326	SIO2	41.90	AL2O3	13.20
327	SIO2	41.60	FEO	15.60
328	SIO2	43.20	FEO	17.10
329	SIO2	42.80	FEO	14.30
330	SIO2	40.90	FEO	15.90
331	SIO2	42.40	FEO	14.40
332	SIO2	51.24	FEO	36.44
333	SIO2	52.54	FEO	31.75
334	SIO2	52.60	FEO	31.84
335	SIO2	52.61	FEO	31.92
336	SIO2	52.18	FEO	33.62
337	SIO2	53.33	FEO	28.70
338	SIO2	52.50	FEO	31.50
339	SIO2	52.87	FEO	29.90
340	SIO2	52.89	FEO	27.65
341	SIO2	53.11	FEO	28.17
342	SIO2	50.63	FEO	37.18
343	SIO2	51.93	FEO	34.44
344	SIO2	54.12	FEO	25.96
345	SIO2	53.04	FEO	27.89
346	SIO2	53.58	FEO	26.72
347	SIO2	54.00	FEO	26.53
348	SIO2	54.48	FEO	24.62
349	SIO2	52.56	FEO	32.48
350	SIO2	57.31	MGO	20.20
351	SIO2	57.48	MGO	20.77
352	SIO2	56.80	MGO	18.97
353	SIO2	57.45	MGO	20.79
354	SIO2	57.07	MGO	20.31
355	SIO2	58.43	MGO	23.61
356	SIO2	58.54	MGO	23.82
357	SIO2	45.97	FEO	12.67
358	SIO2	53.07	MGO	21.78
359	SIO2	41.46	AL2O3	14.24
360	SIO2	38.20	FEO	19.80
361	SIO2	41.01	FEO	21.56
362	SIO2	40.57	FEO	19.70
363	SIO2	49.51	MGO	18.11
364	SIO2	53.92	MGO	18.44
365	SIO2	54.60	MGO	18.90
366	SIO2	54.60	MGO	19.30
367	SIO2	53.20	MGO	17.30
368	SIO2	54.70	MGO	18.30
369	SIO2	41.00	FEO	29.10
370	SIO2	46.40	FEO	17.00
371	SIO2	40.30	MGO	12.50
372	SIO2	43.80	MGO	14.20
373	SIO2	46.00	MGO	14.60
374	SIO2	46.90	MGO	15.80
375	SIO2	43.70	AL2O3	15.10
376	SIO2	47.64	CAO	13.85
377	SIO2	42.52	FEO	16.87
378	SIO2	49.48	MGO	18.02
379	SIO2	43.59	MGO	14.46
380	SIO2	44.83	MGO	16.89
381	SIO2	52.48	FEO	17.34
382	SIO2	55.65	MGO	21.60
383	SIO2	45.73	MGO	12.32
384	SIO2	44.09	FEO	12.96
385	SIO2	52.10	MGO	11.80
386	SIO2	51.53	MGO	20.84
387	SIO2	55.60	AL2O3	12.40
388	SIO2	56.70	FEO	10.40
389	SIO2	56.73	FEO	11.96
390	SIO2	55.20	FEO	10.60
391	SIO2	55.50	FEO	10.10
392	SIO2	55.04	FEO	11.62
393	SIO2	56.40	FEO	10.55
394	SIO2	56.70	MGO	10.10
395	SIO2	52.10	MGO	11.80
396	SIO2	56.90	MGO	10.60
397	SIO2	54.20	FEO	14.00
398	SIO2	53.30	FEO	19.20
399	SIO2	53.80	FEO	15.50
400	SIO2	54.04	MGO	14.62
401	SIO2	51.90	FEO	22.10
402	SIO2	49.60	FEO	18.54
403	SIO2	44.70	FEO	18.96

404	SIO2	56.86	MGO	26.61
405	SIO2	53.41	MGO	15.09
406	SIO2	45.33	FEO	14.61
407	SIO2	45.87	CAO	12.62
408	SIO2	38.04	FEO	21.30
409	SIO2	47.80	MGO	14.58
410	SIO2	41.54	MGO	17.73
411	SIO2	41.52	MGO	17.50
412	SIO2	42.87	MGO	18.26
413	SIO2	53.40	FE2O3	12.79
414	SIO2	53.03	FEO	16.87
415	SIO2	54.29	MGO	15.87
416	SIO2	53.06	FEO	16.06
417	SIO2	43.20	FEO	21.85
418	SIO2	54.63	MGO	19.32
419	SIO2	45.68	MGO	13.39
420	SIO2	51.18	MGO	16.79
421	SIO2	42.50	AL2O3	15.14
422	SIO2	39.60	AL2O3	19.04
423	SIO2	45.01	MGO	13.40
424	SIO2	44.50	AL2O3	12.50
425	SIO2	45.16	FEO	13.54
426	SIO2	45.20	FEO	15.80
427	SIO2	39.29	AL2O3	13.80
428	SIO2	41.95	AL2O3	14.92
429	SIO2	46.49	MGO	12.62
430	SIO2	55.46	MGO	17.83
431	SIO2	42.11	FEO	15.14
432	SIO2	43.01	MGO	14.00
433	SIO2	48.92	MGO	14.32
434	SIO2	45.50	MGO	14.61
435	SIO2	48.32	MGO	14.82
436	SIO2	48.96	MGO	15.69
437	SIO2	44.23	AL2O3	14.62
438	SIO2	44.15	MGO	12.30
439	SIO2	47.14	MGO	14.44
440	SIO2	40.21	AL2O3	12.78
441	SIO2	47.95	MGO	13.33
442	SIO2	46.17	FEO	12.97
443	SIO2	46.30	FEO	12.09
444	SIO2	46.63	MGO	12.03
445	SIO2	46.90	MGO	12.70
446	SIO2	44.00	FEO	13.80
447	SIO2	46.30	FEO	15.40
448	SIO2	46.20	FEO	13.80
449	SIO2	44.12	FEO	14.77
450	SIO2	44.67	FEO	14.76
451	SIO2	44.30	FEO	14.70
452	SIO2	45.97	FEO	12.58
453	SIO2	47.11	FEO	12.40
454	SIO2	49.46	MGO	13.61
455	SIO2	49.70	MGO	14.40
456	SIO2	48.70	MGO	14.20
457	SIO2	50.40	MGO	14.50
459	SIO2	49.90	MGO	13.20
460	SIO2	45.02	MGO	12.37
461	SIO2	49.72	MGO	14.98
462	SIO2	55.20	MGO	21.65
463	SIO2	46.56	MGO	20.58
464	SIO2	45.06	MGO	13.84
465	SIO2	44.94	CAO	13.00
466	SIO2	44.82	CAO	14.43
467	SIO2	44.80	MGO	13.95
468	SIO2	44.74	FEO	13.69
469	SIO2	43.70	CAO	13.00
470	SIO2	43.34	CAO	12.91
471	SIO2	42.52	CAO	13.88
472	SIO2	35.66	FE2O3	13.78
473	SIO2	42.74	CAO	12.72
474	SIO2	40.52	CAO	12.33
475	SIO2	51.50	MGO	16.95
476	SIO2	39.70	MGO	14.66
477	SIO2	57.45	MGO	24.94
478	SIO2	56.34	MGO	23.81
479	SIO2	45.07	AL2O3	13.82
480	SIO2	48.64	MGO	16.42
481	SIO2	42.41	MGO	14.79
482	SIO2	56.10	FE2O3	13.67
483	SIO2	55.38	FE2O3	15.69
484	SIO2	51.86	FE2O3	20.26

485	SIO2	50.50	FE2O3	20.20
486	SIO2	51.94	FEO	19.39
487	SIO2	59.40	FEO	15.10
488	SIO2	54.68	FE2O3	13.98
489	SIO2	55.16	FE2O3	14.02
490	SIO2	43.31	MGO	19.39
491	SIO2	46.93	MGO	14.90
492	SIO2	39.09	AL2O3	15.34
493	SIO2	52.22	MGO	19.20
494	SIO2	46.48	FEO	14.51
495	SIO2	45.80	FEO	19.13
496	SIO2	40.73	FEO	19.92
497	SIO2	45.21	FEO	17.86
498	SIO2	50.18	CAO	16.14
499	SIO2	43.51	FEO	12.87
500	SIO2	43.30	FEO	13.03
501	SIO2	41.38	FEO	13.91
502	SIO2	42.15	FEO	13.99
503	SIO2	42.24	FEO	13.95
504	SIO2	42.43	FEO	14.01
505	SIO2	42.18	FEO	14.21
506	SIO2	43.35	FEO	12.24
507	SIO2	43.63	FEO	12.16
508	SIO2	40.51	FEO	17.16
509	SIO2	42.32	FEO	13.46
510	SIO2	41.89	FEO	14.09
511	SIO2	42.35	FEO	12.53
512	SIO2	42.58	FEO	13.59
513	SIO2	42.36	AL2O3	13.41
514	SIO2	42.06	FEO	14.83
515	SIO2	42.05	FEO	14.36
516	SIO2	41.73	FEO	14.19
517	SIO2	42.48	FEO	14.84
518	SIO2	41.61	FEO	15.03
519	SIO2	42.38	FEO	15.03
520	SIO2	42.36	FEO	13.97
521	SIO2	41.67	FEO	13.84
522	SIO2	42.96	FEO	13.33
523	SIO2	42.36	FEO	14.74
524	SIO2	42.24	AL2O3	12.09
525	SIO2	42.51	FEO	14.01
526	SIO2	42.57	FEO	12.60
527	SIO2	42.42	FEO	17.73
528	SIO2	43.16	FEO	12.70
529	SIO2	43.43	FEO	13.68
530	SIO2	43.01	FEO	14.09
531	SIO2	42.73	FEO	14.36
532	SIO2	43.40	FEO	12.60
533	SIO2	34.41	FEO	26.07
534	SIO2	40.55	FEO	14.42
535	SIO2	39.15	FEO	15.08
536	SIO2	35.17	AL2O3	15.83
537	SIO2	49.72	MGO	14.98
538	SIO2	44.92	AL2O3	15.26
539	SIO2	41.96	FEO	13.34
540	SIO2	55.21	MGO	18.97
541	SIO2	48.64	FEO	14.52
542	SIO2	48.40	FEO	14.82
543	SIO2	43.11	FEO	13.04
544	SIO2	52.42	MGO	15.85
545	SIO2	50.08	MGO	16.31
546	SIO2	53.71	MGO	22.42
547	SIO2	45.63	MGO	19.78
548	SIO2	42.58	CAO	12.15
549	SIO2	44.18	FEO	13.59
550	SIO2	44.29	FEO	13.87
551	SIO2	42.12	FEO	13.23
552	SIO2	42.97	FEO	12.31
553	SIO2	43.95	FEO	15.12
554	SIO2	42.47	FEO	12.92
555	SIO2	44.67	FEO	12.24
556	SIO2	41.73	FEO	13.12
557	SIO2	38.06	FEO	16.03
558	SIO2	50.88	FEO	13.41
559	SIO2	50.41	FEO	10.81
560	SIO2	45.31	FEO	13.60
561	SIO2	41.82	AL2O3	19.33
562	SIO2	50.30	FEO	33.70
563	SIO2	51.50	FEO	35.70
564	SIO2	51.60	FEO	39.70

565	SIO2	52.00	FEO	37.00
566	SIO2	52.00	FEO	36.50
567	SIO2	52.70	FEO	38.90
568	SIO2	53.30	FEO	34.30
569	SIO2	52.10	FEO	41.60
570	SIO2	58.00	MGO	24.50
571	SIO2	58.00	MGO	24.00
572	SIO2	51.00	FEO	35.00
573	SIO2	51.20	FEO	35.60
574	SIO2	52.00	FEO	31.00
575	SIO2	52.00	FEO	30.00
576	SIO2	54.00	FEO	30.50
577	SIO2	49.20	FEO	27.60
578	SIO2	52.00	MGO	17.50
579	SIO2	48.00	FEO	18.00
580	SIO2	48.00	FEO	19.50
581	SIO2	42.00	FEO	25.00
582	SIO2	46.40	FEO	24.44
583	SIO2	52.00	FEO	21.50
584	SIO2	56.80	MGO	15.50
585	SIO2	50.50	FEO	21.50
586	SIO2	39.65	FEO	15.46
587	SIO2	40.30	AL2O3	14.17
588	SIO2	41.53	FEO	13.22
589	SIO2	39.50	AL2O3	14.14
590	SIO2	41.34	AL2O3	12.76
591	SIO2	40.14	AL2O3	13.92
592	SIO2	54.82	MGO	17.60
593	SIO2	44.09	FEO	18.83
594	SIO2	43.82	AL2O3	15.79
595	SIO2	55.44	FE2O3	16.77
596	SIO2	53.50	FE2O3	14.50
597	SIO2	53.63	FEO	12.12
598	SIO2	50.82	MGO	10.30
599	SIO2	51.63	AL2O3	10.72
600	SIO2	55.62	FE2O3	12.99
601	SIO2	56.89	MGO	15.53
602	SIO2	52.86	FEO	15.23
603	SIO2	58.04	MGO	11.71
604	SIO2	55.19	AL2O3	9.94
605	SIO2	55.36	AL2O3	12.16
606	SIO2	49.95	FE2O3	16.93
607	SIO2	46.30	CAO	15.60
608	SIO2	45.76	MGO	14.08
609	SIO2	49.58	MGO	15.41
610	SIO2	48.00	FEO	26.11
611	SIO2	51.10	FEO	22.18
612	SIO2	46.18	MGO	25.05
613	SIO2	53.40	FEO	17.40
614	SIO2	56.92	MGO	20.99
615	SIO2	56.44	MGO	21.12
616	SIO2	55.01	MGO	23.85
617	SIO2	44.09	FEO	20.29
618	SIO2	45.71	AL2O3	12.98
619	SIO2	46.30	MGO	15.60
620	SIO2	49.32	MGO	16.12
621	SIO2	48.20	FEO	16.70
622	SIO2	53.04	MGO	18.46
623	SIO2	49.58	MGO	15.41
624	SIO2	48.00	FEO	26.11
625	SIO2	50.10	FEO	22.86
626	SIO2	50.54	MGO	14.02
627	SIO2	43.70	FEO	26.53
628	SIO2	50.70	FEO	26.63
629	SIO2	54.97	MGO	22.11
630	SIO2	51.59	MGO	16.92
631	SIO2	42.24	FEO	16.06
632	SIO2	49.12	FEO	16.70
633	SIO2	49.92	FEO	18.46
634	SIO2	52.59	FEO	11.80
635	SIO2	38.81	FEO	21.72
636	SIO2	44.32	FEO	16.88
637	SIO2	43.58	MGO	18.30
638	SIO2	45.00	MGO	12.60
639	SIO2	47.21	MGO	12.82
640	SIO2	45.68	MGO	13.33
641	SIO2	45.44	AL2O3	12.49
642	SIO2	44.40	MGO	13.58
643	SIO2	44.35	CAO	12.72
644	SIO2	44.30	FEO	11.70

645	SIO2	44.26	MGO	13.21
646	SIO2	44.12	CAO	11.97
647	SIO2	43.43	AL2O3	12.30
648	SIO2	43.30	MGO	11.94
649	SIO2	39.60	FEO	12.15
650	SIO2	38.91	CAO	12.34
651	SIO2	44.43	FEO	13.47
652	SIO2	59.17	MGO	29.07
653	SIO2	57.11	MGO	25.23
654	SIO2	57.42	MGO	24.09
655	SIO2	53.10	MGO	21.06
656	SIO2	56.02	MGO	21.44
657	SIO2	56.13	MGO	23.66
658	SIO2	57.61	MGO	25.43
659	SIO2	56.54	MGO	23.83
660	SIO2	58.22	MGO	27.27
661	SIO2	55.97	MGO	21.55
662	SIO2	61.70	MGO	29.90
663	SIO2	55.64	MGO	22.09
664	SIO2	40.64	AL2O3	13.88
665	SIO2	48.20	MGO	19.58
666	SIO2	43.50	FEO	18.20
667	SIO2	43.70	FEO	17.80
668	SIO2	58.74	MGO	24.63
669	SIO2	58.22	MGO	23.97
670	SIO2	48.38	MGO	20.78
671	SIO2	55.02	MGO	20.36
672	SIO2	43.35	MGO	14.33
673	SIO2	40.52	CAO	12.33
674	SIO2	48.42	MGO	21.32
682	SIO2	53.20	MGO	11.12
683	SIO2	50.15	MGO	15.90
684	SIO2	48.15	MGO	14.60
685	SIO2	48.08	AL2O3	13.00
686	SIO2	47.55	AL2O3	13.82
687	SIO2	47.55	AL2O3	15.28
688	SIO2	46.74	AL2O3	13.45
689	SIO2	38.89	FEO	21.88
690	SIO2	41.30	AL2O3	15.60
691	SIO2	43.03	AL2O3	26.65
692	SIO2	42.99	FEO	14.03
693	SIO2	52.51	MGO	18.21
694	SIO2	52.87	MGO	20.52
695	SIO2	52.40	MGO	19.70
696	SIO2	40.10	AL2O3	14.71
697	SIO2	53.85	MGO	14.73
698	SIO2	46.78	MGO	17.28
699	SIO2	44.88	MGO	13.63
718	SIO2	45.94	FE2O3	14.63
719	SIO2	45.15	FEO	12.81
720	SIO2	39.20	AL2O3	15.50
721	SIO2	41.56	AL2O3	13.25
722	SIO2	41.47	AL2O3	13.30
723	SIO2	41.38	AL2O3	13.44
724	SIO2	40.82	AL2O3	14.21
725	SIO2	40.62	AL2O3	14.74
726	SIO2	39.58	AL2O3	14.15
727	SIO2	39.15	AL2O3	14.02
728	SIO2	49.63	FEO	16.74
729	SIO2	38.26	FEO	22.66
730	SIO2	38.03	FEO	23.72
731	SIO2	54.70	FEO	20.40
732	SIO2	59.30	MGO	30.00
733	SIO2	37.48	FEO	29.88
734	SIO2	59.97	AL2O3	13.29
735	SIO2	53.26	MGO	19.21
736	SIO2	50.98	FEO	15.69
737	SIO2	41.63	FE2O3	15.41
738	SIO2	47.27	MGO	13.11
739	SIO2	40.17	CAO	12.41
740	SIO2	43.04	AL2O3	12.38
741	SIO2	49.95	FEO	16.71
742	SIO2	57.98	MGO	18.98
743	SIO2	55.25	MGO	17.57
744	SIO2	53.87	MGO	17.09
745	SIO2	47.95	MGO	13.02
746	SIO2	40.62	MGO	14.03
747	SIO2	46.19	MGO	18.71
748	SIO2	44.35	MGO	17.26
749	SIO2	44.90	MGO	15.22

750	SIO2	46.06	MGO	12.81
751	SIO2	43.46	FEO	14.53
752	SIO2	44.77	FEO	14.17
753	SIO2	61.55	MGO	39.14
754	SIO2	51.01	FEO	17.62
755	SIO2	42.00	FEO	15.20
756	SIO2	49.72	MGO	14.08
757	SIO2	50.58	FE2O3	16.15
758	SIO2	42.38	FEO	13.80
759	SIO2	37.79	FEO	15.99
760	SIO2	56.35	MGO	24.97
761	SIO2	43.50	AL2O3	16.00
762	SIO2	49.16	FEO	14.48
763	SIO2	49.55	FEO	37.03
764	SIO2	58.48	MGO	29.25
765	SIO2	53.16	MGO	30.03
766	SIO2	41.72	AL2O3	15.86
767	SIO2	51.30	FEO	18.50
768	SIO2	54.56	FEO	16.12
769	SIO2	53.12	FEO	22.46
770	SIO2	44.29	AL2O3	16.50
771	SIO2	40.60	AL2O3	14.10
772	SIO2	57.13	MGO	21.86
773	SIO2	55.82	MGO	22.61
774	SIO2	41.67	FEO	16.28
775	SIO2	38.84	AL2O3	13.70
776	SIO2	42.00	FEO	13.50
777	SIO2	43.00	FEO	12.00
778	SIO2	43.00	FEO	14.00
779	SIO2	50.00	MGO	13.50
780	SIO2	45.00	MGO	16.50
781	SIO2	47.47	CAO	14.05
783	SIO2	46.10	FEO	40.10
784	SIO2	47.40	FEO	39.30
785	SIO2	48.00	FEO	35.10
786	SIO2	40.00	AL2O3	14.09
787	SIO2	40.96	AL2O3	34.02
788	SIO2	41.72	AL2O3	15.86
789	SIO2	45.72	MGO	12.37
790	SIO2	46.72	MGO	14.43
791	SIO2	44.95	MGO	14.12
792	SIO2	49.74	MGO	20.44
793	SIO2	42.83	FEO	14.55
794	SIO2	47.73	FEO	23.25
795	SIO2	48.83	FEO	21.77
796	SIO2	45.50	MGO	20.63
797	SIO2	39.23	AL2O3	14.38
798	SIO2	38.63	CAO	12.81
799	SIO2	46.12	MGO	21.22
800	SIO2	46.26	MGO	19.03
801	SIO2	45.48	MGO	12.49
802	SIO2	47.54	MGO	13.25
803	SIO2	54.70	MGO	18.55
804	SIO2	45.79	MGO	13.13
805	SIO2	44.07	FEO	12.70
806	SIO2	42.25	AL2O3	19.26
807	SIO2	50.26	MGO	12.28
808	SIO2	49.56	MGO	11.04
809	SIO2	53.13	FE2O3	14.30
810	SIO2	49.78	MGO	14.94
811	SIO2	50.48	MGO	15.16
812	SIO2	49.77	MGO	15.44
813	SIO2	50.46	FEO	15.79
814	SIO2	48.98	MGO	14.23
815	SIO2	50.35	MGO	15.84
816	SIO2	49.96	MGO	15.67
817	SIO2	50.90	MGO	16.60
818	SIO2	50.70	MGO	15.94
819	SIO2	51.72	MGO	16.87
820	SIO2	43.48	MGO	14.03
821	SIO2	50.49	MGO	15.27
822	SIO2	50.74	MGO	15.77
823	SIO2	50.23	MGO	18.01
824	SIO2	49.37	MGO	15.09
825	SIO2	46.23	MGO	13.54
826	SIO2	43.11	FEO	14.02
827	SIO2	57.31	MGO	22.80
828	SIO2	51.33	MGO	20.05
829	SIO2	40.28	AL2O3	15.48
830	SIO2	37.90	FE2O3	25.30

831	SIO2	34.50	FE2O3	26.20
832	SIO2	46.68	AL2O3	14.37
833	SIO2	46.48	MGO	16.52
834	SIO2	44.53	MGO	18.78
835	SIO2	42.73	AL2O3	22.73
838	SIO2	44.22	AL2O3	23.79
839	SIO2	50.75	MGO	14.12
840	SIO2	54.80	FE2O3	11.72
841	SIO2	39.85	AL2O3	14.74
842	SIO2	39.66	MGO	14.56
843	SIO2	45.96	AL2O3	14.84
844	SIO2	43.18	AL2O3	16.84
845	SIO2	44.60	MGO	15.55
846	SIO2	45.88	AL2O3	14.05
847	SIO2	39.24	AL2O3	14.14
848	SIO2	41.41	MGO	13.21
849	SIO2	41.16	MGO	13.54
850	SIO2	41.05	FEO	13.74
851	SIO2	40.74	MGO	12.92
852	SIO2	42.83	MGO	15.39
853	SIO2	40.46	MGO	13.93
854	SIO2	41.65	MGO	14.96
855	SIO2	40.64	MGO	13.84
856	SIO2	42.16	FEO	14.75
857	SIO2	44.22	MGO	14.73
858	SIO2	42.92	MGO	13.45
859	SIO2	44.61	MGO	14.14
860	SIO2	45.76	FEO	14.52
861	SIO2	42.32	FEO	14.20
862	SIO2	44.20	FEO	14.21
863	SIO2	43.21	FEO	13.63
864	SIO2	43.81	FEO	13.73
865	SIO2	44.33	FEO	14.27
866	SIO2	45.50	MGO	14.36
868	SIO2	52.21	FEO	17.19
869	SIO2	49.24	MGO	15.84
870	SIO2	51.79	FEO	31.91
871	SIO2	48.96	FEO	38.16
872	SIO2	55.44	FEO	23.64
873	SIO2	44.89	MGO	18.09
874	SIO2	54.15	MGO	20.42
875	SIO2	43.70	AL2O3	16.11
876	SIO2	47.00	MGO	13.90
877	SIO2	47.56	MGO	13.15
878	SIO2	48.00	MGO	12.60
879	SIO2	48.08	MGO	13.43
880	SIO2	48.00	MGO	12.70
881	SIO2	54.84	MGO	18.64
882	SIO2	54.42	MGO	17.86
883	SIO2	39.10	FEO	25.49
884	SIO2	38.78	FEO	28.08
885	SIO2	34.38	FEO	26.72
886	SIO2	42.70	FEO	13.78
887	SIO2	42.09	MGO	16.16
888	SIO2	49.40	FE2O3	19.57
889	SIO2	50.85	FEO	19.55
890	SIO2	51.40	FEO	19.95
891	SIO2	57.46	FE2O3	16.85
892	SIO2	52.40	FE2O3	19.05
893	SIO2	50.35	FEO	19.45
894	SIO2	50.10	FE2O3	18.85
895	SIO2	50.70	FE2O3	18.30
896	SIO2	52.27	FE2O3	17.48
897	SIO2	52.27	FE2O3	17.12
898	SIO2	52.00	FEO	17.65
899	SIO2	59.41	FEO	15.11
900	SIO2	63.65	FE2O3	14.18
901	SIO2	59.90	FE2O3	16.57
902	SIO2	52.85	FE2O3	18.55
903	SIO2	55.65	MGO	13.09
904	SIO2	55.10	AL2O3	10.97
905	SIO2	55.35	AL2O3	10.94
906	SIO2	54.41	AL2O3	10.93
907	SIO2	54.56	FEO	14.41
908	SIO2	44.53	MGO	12.90
909	SIO2	56.52	FEO	10.61
910	SIO2	52.90	MGO	15.18
911	SIO2	49.86	FEO	14.32
912	SIO2	45.19	FEO	12.93
913	SIO2	44.32	FEO	13.12

914	SIO2	42.81	FEO	14.10
915	SIO2	46.28	MGO	12.96
916	SIO2	43.93	AL2O3	12.18
917	SIO2	45.99	FEO	13.79
918	SIO2	41.59	FEO	14.57
919	SIO2	50.41	FEO	10.81
920	SIO2	55.02	FE2O3	10.91
922	SIO2	44.80	FEO	15.00
923	SIO2	42.30	FEO	16.20
924	SIO2	44.20	FEO	15.05
925	SIO2	41.90	FEO	17.00
926	SIO2	41.40	FEO	17.40
927	SIO2	41.00	FEO	12.10
928	SIO2	41.00	FEO	17.30
929	SIO2	41.80	FEO	17.60
930	SIO2	43.40	FEO	15.50
931	SIO2	44.30	FEO	15.60
932	SIO2	41.60	FEO	16.30
933	SIO2	41.40	FEO	16.80
934	SIO2	41.00	FEO	17.60
935	SIO2	40.00	FEO	18.40
936	SIO2	42.10	FEO	18.40
937	SIO2	41.00	FEO	20.40
938	SIO2	35.52	AL2O3	19.57
939	SIO2	37.02	AL2O3	17.29
940	SIO2	37.58	FE2O3	20.75
941	SIO2	37.62	AL2O3	16.77
942	SIO2	42.35	MGO	14.33
943	SIO2	59.06	AL2O3	12.38
944	SIO2	38.24	AL2O3	15.16
945	SIO2	39.12	AL2O3	14.67
946	SIO2	58.74	MGO	24.63
947	SIO2	57.60	MGO	24.16
948	SIO2	57.34	MGO	24.05
949	SIO2	56.26	MGO	23.59
950	SIO2	45.44	AL2O3	12.49
951	SIO2	43.43	AL2O3	12.30
952	SIO2	44.26	MGO	13.21
953	SIO2	44.30	FEO	11.70
954	SIO2	43.30	MGO	11.94
955	SIO2	38.91	CAO	12.34
956	SIO2	45.68	MGO	13.33
957	SIO2	44.12	CAO	11.97
958	SIO2	44.35	CAO	12.72
959	SIO2	44.40	MGO	13.58
960	SIO2	47.21	MGO	12.82
961	SIO2	39.60	FEO	12.15
962	SIO2	48.20	AL2O3	11.51
963	SIO2	52.40	MGO	14.33
964	SIO2	47.50	MGO	14.43
965	SIO2	43.50	MGO	14.01
966	SIO2	36.98	FEO	16.60
967	SIO2	36.91	FEO	17.94
968	SIO2	36.44	FEO	17.32
969	SIO2	37.71	FEO	19.50
970	SIO2	36.64	FEO	18.34
971	SIO2	36.59	FEO	16.99
972	SIO2	36.96	FEO	19.25
973	SIO2	36.52	FEO	18.32
974	SIO2	40.26	FEO	22.16
975	SIO2	40.30	FEO	19.75
979	SIO2	52.19	MGO	14.54
980	SIO2	50.47	MGO	17.94
981	SIO2	40.09	FEO	11.78
982	SIO2	40.69	MGO	14.34
983	SIO2	39.48	CAO	13.65
984	SIO2	46.54	AL2O3	13.78
985	SIO2	46.02	AL2O3	13.16
986	SIO2	45.86	FEO	13.03
987	SIO2	44.16	FEO	13.19
988	SIO2	43.20	FEO	14.26
989	SIO2	58.34	MGO	21.77
990	SIO2	55.64	MGO	20.52
991	SIO2	47.99	FEO	11.25
992	SIO2	56.00	MNO	20.50
993	SIO2	52.70	MGO	19.26
994	SIO2	53.50	MGO	23.65
995	SIO2	51.45	MGO	22.78
996	SIO2	56.35	MGO	24.97
997	SIO2	57.12	MGO	24.66

998	SIO2	55.53	MGO	24.40
999	SIO2	55.93	MGO	21.28
1000	SIO2	57.00	MGO	22.82
1001	SIO2	57.98	MGO	24.39
1002	SIO2	55.89	MGO	21.20
1003	SIO2	58.36	MGO	23.10
1004	SIO2	57.81	MGO	25.44
1005	SIO2	56.00	MGO	20.52
1006	SIO2	51.88	MGO	16.36
1007	SIO2	51.47	MGO	17.20
1008	SIO2	52.80	CAO	12.20
1009	SIO2	52.20	AL2O3	11.39
1010	SIO2	50.40	AL2O3	11.50
1011	SIO2	49.82	AL2O3	12.30
1012	SIO2	46.40	AL2O3	16.30
1013	SIO2	54.86	MGO	15.03
1014	SIO2	47.54	FEO	47.25
1015	SIO2	42.92	FEO	11.98
1016	SIO2	42.70	FEO	13.78
1017	SIO2	46.87	CAO	12.82
1018	SIO2	47.40	MGO	14.61
1019	SIO2	49.78	MGO	15.78
1020	SIO2	49.54	MGO	15.64
1021	SIO2	47.09	CAO	13.51
1022	SIO2	40.00	AL2O3	14.09
1023	SIO2	47.42	MGO	12.83
1024	SIO2	43.90	FEO	11.54
1025	SIO2	43.26	FEO	12.63
1026	SIO2	41.96	FEO	14.40
1027	SIO2	41.18	AL2O3	15.89
1028	SIO2	49.63	MGO	16.23
1029	SIO2	44.67	FEO	12.85
1030	SIO2	43.93	MGO	12.85
1031	SIO2	41.88	CAO	11.69
1032	SIO2	45.24	FEO	12.51
1033	SIO2	59.92	MGO	24.36
1034	SIO2	58.60	MGO	24.66
1035	SIO2	57.57	MGO	22.59
1036	SIO2	53.23	MGO	21.17
1037	SIO2	51.44	MGO	18.75
1038	SIO2	49.53	MGO	14.64
1039	SIO2	41.03	FEO	16.10
1040	SIO2	36.01	FEO	16.09
1041	SIO2	54.81	MGO	13.52
1042	SIO2	44.56	MGO	22.37
1043	SIO2	48.00	FEO	19.30
1044	SIO2	47.80	FEO	26.60
1045	SIO2	55.54	MGO	25.40
1046	SIO2	56.40	MGO	26.85
1047	SIO2	56.16	MGO	23.07
1048	SIO2	56.44	MGO	22.84
1049	SIO2	54.03	MGO	22.01
1050	SIO2	53.60	FEO	30.10
1051	SIO2	43.90	FEO	20.70
1052	SIO2	53.20	FEO	30.20
1053	SIO2	41.40	FEO	21.00
1054	SIO2	52.25	FEO	28.20
1055	SIO2	41.90	FEO	21.35
1056	SIO2	54.55	FEO	27.50
1057	SIO2	43.60	FEO	19.65
1058	SIO2	53.60	FEO	26.40
1059	SIO2	43.85	FEO	19.75
1060	SIO2	54.20	FEO	26.15
1061	SIO2	41.80	FEO	20.10
1062	SIO2	54.80	FEO	23.80
1063	SIO2	45.70	FEO	16.80
1064	SIO2	55.00	FEO	23.60
1065	SIO2	42.10	FEO	15.40
1066	SIO2	56.55	FEO	21.45
1067	SIO2	42.80	AL2O3	16.00
1068	SIO2	47.16	MGO	19.06
1069	SIO2	47.50	MGO	17.70
1070	SIO2	49.01	FEO	44.99
1071	SIO2	49.33	FEO	40.94
1072	SIO2	51.58	FEO	34.40
1073	SIO2	51.95	FEO	33.70
1074	SIO2	51.79	FEO	34.38
1075	SIO2	52.28	FEO	31.90
1076	SIO2	55.27	MGO	19.18
1077	SIO2	55.74	MGO	18.55

1078	SIO2	55.10	MGO	17.00
1079	SIO2	60.00	MGO	33.40
1080	SIO2	58.70	MGO	26.00
1081	SIO2	58.00	MGO	32.50
1082	SIO2	57.50	MGO	25.40
1083	SIO2	56.40	MGO	27.80
1084	SIO2	56.70	MGO	23.20
1085	SIO2	49.10	MGO	19.80
1086	SIO2	45.70	MGO	15.60
1087	SIO2	51.20	MGO	20.00
1088	SIO2	46.30	MGO	14.80
1089	SIO2	48.80	MGO	18.80
1090	SIO2	45.80	MGO	15.50
1091	SIO2	49.50	MGO	18.80
1092	SIO2	44.20	AL2O3	15.90
1093	SIO2	50.80	FEO	19.70
1094	SIO2	44.00	AL2O3	15.40
1095	SIO2	49.00	FEO	19.50
1096	SIO2	44.50	FEO	15.80
1097	SIO2	49.90	FEO	20.60
1098	SIO2	45.80	FEO	14.70
1099	SIO2	48.40	FEO	21.10
1100	SIO2	45.10	FEO	14.80
1101	SIO2	56.20	MGO	21.20
1102	SIO2	47.20	MGO	18.00
1103	SIO2	55.10	MGO	20.50
1104	SIO2	46.30	MGO	15.30
1105	SIO2	53.00	MGO	20.50
1106	SIO2	45.10	MGO	14.30
1107	SIO2	52.20	FEO	20.20
1108	SIO2	43.70	AL2O3	14.40
1109	SIO2	51.50	FEO	19.00
1110	SIO2	44.60	FEO	16.20
1111	SIO2	53.40	FEO	21.20
1112	SIO2	47.40	MGO	15.80
1113	SIO2	52.30	FEO	18.90
1114	SIO2	45.50	FEO	15.30
1115	SIO2	52.10	FEO	21.50
1116	SIO2	46.50	FEO	16.60
1117	SIO2	54.90	FEO	22.40
1118	SIO2	45.20	FEO	15.60
1119	SIO2	54.10	FEO	22.50
1120	SIO2	47.90	FEO	13.20
1121	SIO2	54.30	FEO	22.90
1122	SIO2	43.80	FEO	20.30
1123	SIO2	54.20	FEO	24.00
1124	SIO2	46.00	FEO	16.40
1125	SIO2	51.40	FEO	23.10
1126	SIO2	43.20	FEO	14.20
1127	SIO2	51.30	FEO	24.20
1128	SIO2	44.60	MGO	19.38
1129	SIO2	53.50	FEO	25.50
1130	SIO2	43.80	FEO	18.50
1131	SIO2	52.50	FEO	26.80
1132	SIO2	42.10	FEO	19.60
1133	SIO2	52.00	FEO	24.90
1134	SIO2	45.90	FEO	19.00
1135	SIO2	52.30	FEO	25.10
1136	SIO2	44.10	FEO	20.20
1137	SIO2	50.50	FEO	26.10
1138	SIO2	47.00	FEO	19.00
1139	SIO2	52.60	FEO	26.80
1140	SIO2	44.50	FEO	16.90
1141	SIO2	51.10	FEO	28.40
1142	SIO2	45.00	FEO	19.80
1143	SIO2	51.30	FEO	27.00
1144	SIO2	47.40	FEO	17.50
1145	SIO2	49.60	FEO	32.00
1146	SIO2	44.10	FEO	22.90
1147	SIO2	49.20	FEO	34.20
1148	SIO2	39.90	FEO	24.30
1149	SIO2	52.10	FEO	25.00
1150	SIO2	50.80	FEO	26.30
1151	SIO2	52.20	FEO	26.80
1152	SIO2	51.40	FEO	26.30
1153	SIO2	52.07	FEO	22.36
1154	SIO2	45.15	FEO	13.52
1155	SIO2	55.00	MGO	20.00
1156	SIO2	48.90	MGO	16.80
1157	SIO2	57.20	MGO	18.60

1158	SIO2	51.20	MGO	16.10
1159	SIO2	55.50	MGO	16.90
1160	SIO2	49.50	FEO	17.70
1161	SIO2	54.70	MGO	14.50
1162	SIO2	46.30	FEO	16.60
1163	SIO2	53.40	MGO	16.00
1164	SIO2	47.10	FEO	17.40
1165	SIO2	52.20	FEO	16.10
1166	SIO2	45.70	FEO	18.60
1167	SIO2	51.30	FEO	16.50
1168	SIO2	44.80	FEO	21.80
1169	SIO2	55.80	MGO	18.70
1170	SIO2	56.60	MGO	13.20
1171	SIO2	54.80	MGO	18.30
1172	SIO2	54.80	FEO	15.90
1173	SIO2	53.60	MGO	17.20
1174	SIO2	55.80	AL2O3	12.60
1175	SIO2	54.00	MGO	16.90
1176	SIO2	54.60	FEO	14.50
1177	SIO2	54.04	MGO	14.62
1178	SIO2	55.04	FEO	11.62
1179	SIO2	51.60	MGO	16.00
1180	SIO2	55.30	FEO	14.00
1181	SIO2	52.20	MGO	16.30
1182	SIO2	55.40	FEO	14.20
1183	SIO2	53.90	MGO	16.50
1184	SIO2	57.40	MGO	14.80
1185	SIO2	52.50	MGO	14.50
1186	SIO2	55.70	AL2O3	12.40
1187	SIO2	43.50	AL2O3	14.80
1188	SIO2	54.50	FEO	13.70
1189	SIO2	46.90	FEO	18.20
1190	SIO2	53.80	FEO	17.70
1191	SIO2	47.40	MGO	16.00
1192	SIO2	45.40	FEO	15.70
1193	SIO2	52.80	MGO	15.70
1194	SIO2	54.60	FEO	15.40
1195	SIO2	53.50	FEO	14.00
1196	SIO2	53.60	FEO	18.50
1197	SIO2	49.40	FEO	18.80
1198	SIO2	52.20	MGO	15.00
1199	SIO2	52.80	FEO	14.80
1200	SIO2	49.40	FEO	19.20
1201	SIO2	53.60	MGO	16.90
1202	SIO2	51.50	MNO	13.20
1203	SIO2	49.74	MNO	13.79
1204	SIO2	55.70	MGO	21.20
1205	SIO2	53.50	MGO	14.60
1206	SIO2	54.40	MGO	15.40
1207	SIO2	54.20	MGO	14.60
1208	SIO2	53.90	MGO	14.60
1209	SIO2	53.80	MGO	14.50
1210	SIO2	54.40	MGO	14.70
1211	SIO2	53.30	ZNO	13.70
1212	SIO2	52.80	MGO	12.50
1213	SIO2	53.00	MGO	11.00
1214	SIO2	48.15	CAO	12.16
1215	SIO2	47.32	CAO	13.21
1216	SIO2	42.07	AL2O3	15.05
1217	SIO2	41.81	CAO	13.52
1218	SIO2	40.10	FE2O3	13.58
1219	SIO2	59.06	AL2O3	12.38
1220	SIO2	44.06	FEO	14.40
1221	SIO2	41.86	AL2O3	14.31
1222	SIO2	58.88	MGO	24.24
1223	SIO2	51.09	MGO	23.06
1224	SIO2	52.21	MGO	24.09
1225	SIO2	38.12	AL2O3	17.21
1226	SIO2	51.90	MGO	16.10
1227	SIO2	44.35	FEO	15.65
1231	SIO2	55.83	MGO	16.82
1232	SIO2	54.82	MGO	15.11
1233	SIO2	54.30	MGO	20.50
1234	SIO2	58.55	MGO	24.55
1235	SIO2	58.20	MGO	25.35
1236	SIO2	55.96	MGO	20.17
1237	SIO2	55.96	MGO	22.62
1238	SIO2	54.20	MGO	22.82
1239	SIO2	53.60	MGO	20.49
1240	SIO2	52.68	MGO	17.17

1241	SIO2	52.08	FEO	15.95
1242	SIO2	46.72	MGO	14.17
1243	SIO2	46.00	FEO	15.61
1244	SIO2	40.86	MGO	16.25
1245	SIO2	56.33	MGO	21.45
1246	SIO2	40.40	FEO	18.16
1247	SIO2	56.81	MGO	20.83
1248	SIO2	54.80	FE2O3	10.40
1251	SIO2	54.20	MGO	14.80
1252	SIO2	53.30	FEO	26.30
1253	SIO2	51.70	FEO	35.20
1254	SIO2	52.00	MGO	19.70
1255	SIO2	48.30	MGO	15.20
1256	SIO2	55.02	MGO	20.36
1257	SIO2	41.00	FEO	25.70
1258	SIO2	38.50	FEO	18.50
1259	SIO2	42.00	FEO	18.80
1260	SIO2	39.50	FEO	18.00
1261	SIO2	41.00	FEO	17.20
1262	SIO2	42.00	FEO	16.10
1263	SIO2	44.50	FEO	15.70
1264	SIO2	45.50	CAO	12.50
1265	SIO2	44.00	FEO	17.50
1266	SIO2	38.00	FEO	18.30
1267	SIO2	42.00	FEO	21.80
1268	SIO2	43.00	FEO	19.70
1269	SIO2	42.00	FEO	19.30
1270	SIO2	38.00	FEO	21.50
1271	SIO2	38.00	FEO	18.80
1272	SIO2	38.00	FEO	19.70
1273	SIO2	58.22	MGO	23.97
1274	SIO2	56.38	MGO	21.74
1275	SIO2	56.01	MGO	20.99
1276	SIO2	55.90	MGO	22.96
1277	SIO2	54.75	MGO	22.54
1278	SIO2	53.42	MGO	18.22
1279	SIO2	49.33	MGO	17.44
1280	SIO2	48.38	MGO	20.76
1281	SIO2	39.75	AL2O3	17.72
1282	SIO2	39.17	AL2O3	14.37
1283	SIO2	36.13	FEO	19.99
1284	SIO2	45.21	FEO	14.85
1285	SIO2	42.15	FEO	12.89
1286	SIO2	44.69	AL2O3	19.61
1287	SIO2	50.59	MGO	14.46
1288	SIO2	48.20	MGO	16.57
1289	SIO2	46.70	MGO	17.31
1290	SIO2	46.60	CAO	11.98
1291	SIO2	45.36	FEO	12.47
1292	SIO2	43.96	FEO	13.22
1293	SIO2	42.61	AL2O3	14.29
1294	SIO2	44.25	MGO	13.60
1295	SIO2	41.50	MGO	15.89
1296	SIO2	52.42	MGO	25.56
1297	SIO2	46.46	MGO	12.35
1298	SIO2	42.05	MGO	13.48
1299	SIO2	43.90	MGO	18.91
1300	SIO2	48.10	MGO	20.60
1301	SIO2	48.38	MGO	20.78
1302	SIO2	41.50	MGO	19.40
1303	SIO2	45.69	MGO	18.79
1304	SIO2	41.90	MGO	21.95
1305	SIO2	51.75	MGO	18.97
1306	SIO2	42.01	MGO	18.27
1307	SIO2	39.37	MGO	21.46
1308	SIO2	42.08	MGO	16.50
1309	SIO2	41.34	FEO	17.14
1310	SIO2	56.40	MGO	21.82
1311	SIO2	56.04	MGO	20.63
1312	SIO2	56.28	MGO	22.22
1313	SIO2	56.97	MGO	21.95
1314	SIO2	53.58	MGO	17.57
1315	SIO2	54.07	MGO	17.88
1316	SIO2	54.30	MGO	17.71
1317	SIO2	52.79	MGO	15.50
1318	SIO2	52.94	MGO	15.02
1319	SIO2	49.66	MGO	14.50
1320	SIO2	49.90	MGO	13.09
1321	SIO2	52.14	MGO	15.52
1322	SIO2	37.70	CAO	16.86

1323	SIO2	37.86	CAO	14.96
1324	SIO2	40.18	MGO	14.87
1325	SIO2	55.26	MGO	20.97
1326	SIO2	56.00	MGO	20.37
1327	SIO2	44.71	AL2O3	16.76
1328	SIO2	48.55	MGO	14.81
1329	SIO2	45.44	MGO	13.04
1330	SIO2	48.17	MGO	13.37
1331	SIO2	47.81	FEO	13.34
1332	SIO2	43.92	FEO	13.36
1333	SIO2	46.62	FEO	13.54
1334	SIO2	43.72	FEO	14.22
1335	SIO2	45.19	FEO	14.50
1336	SIO2	45.93	FEO	16.15
1337	SIO2	39.56	FEO	23.18
1340	SIO2	43.95	MGO	13.73
1341	SIO2	57.70	MGO	21.12
1342	SIO2	40.20	MGO	14.90
1343	SIO2	56.50	MGO	19.22
1344	SIO2	40.15	FEO	13.51
1345	SIO2	47.15	MGO	12.76
1346	SIO2	48.20	FEO	10.60
1347	SIO2	47.60	MGO	12.92
1348	SIO2	48.35	MGO	14.09
1349	SIO2	47.60	MGO	11.94
1350	SIO2	44.42	MGO	16.10
1351	SIO2	42.78	MGO	12.45
1352	SIO2	46.84	MGO	17.81
1353	SIO2	40.60	AL2O3	15.52
1354	SIO2	41.12	AL2O3	15.51
1355	SIO2	42.94	MGO	14.82
1356	SIO2	42.52	MGO	14.92
1357	SIO2	41.42	AL2O3	14.34
1358	SIO2	41.80	AL2O3	13.11
1359	SIO2	39.81	AL2O3	13.78
1360	SIO2	40.94	AL2O3	13.14
1361	SIO2	39.99	AL2O3	13.81
1362	SIO2	40.08	AL2O3	13.81
1363	SIO2	44.10	MGO	17.60
1364	SIO2	49.79	MGO	16.70
1365	SIO2	48.77	MGO	14.74
1366	SIO2	45.75	MGO	12.63
1367	SIO2	43.50	MGO	14.25
1368	SIO2	44.38	AL2O3	17.32
1369	SIO2	38.84	FEO	22.48
1370	SIO2	47.28	MGO	14.13
1371	SIO2	44.08	MGO	14.79
1372	SIO2	41.32	MGO	15.29
1373	SIO2	48.31	MGO	14.51
1374	SIO2	45.78	FEO	16.12
1375	SIO2	44.38	FEO	13.96
1376	SIO2	42.52	FEO	13.00
1377	SIO2	41.70	FEO	17.57
1378	SIO2	40.50	FEO	17.71
1379	SIO2	40.50	FEO	17.16
1380	SIO2	39.78	FEO	19.36
1381	SIO2	37.10	FEO	26.85
1382	SIO2	42.82	AL2O3	14.27
1383	SIO2	43.19	AL2O3	17.77
1384	SIO2	49.12	AL2O3	13.44
1385	SIO2	49.27	FEO	23.00
1386	SIO2	51.22	FE2O3	23.75
1387	SIO2	52.22	FE2O3	28.15
1388	SIO2	40.42	MGO	14.23
1389	SIO2	41.92	FEO	15.62
1390	SIO2	39.25	AL2O3	17.48
1391	SIO2	41.41	AL2O3	13.56
1392	SIO2	40.75	AL2O3	13.85
1393	SIO2	42.11	MGO	14.38
1394	SIO2	48.80	MGO	15.10
1395	SIO2	48.30	MGO	15.80
1396	SIO2	48.70	MGO	15.30
1397	SIO2	57.60	MGO	23.96
1398	SIO2	59.56	MGO	24.31
1399	SIO2	57.29	MGO	23.87
1400	SIO2	55.06	MGO	23.98
1401	SIO2	42.80	MGO	14.24
1402	SIO2	41.12	MGO	18.18
1403	SIO2	39.57	AL2O3	16.29
1404	SIO2	46.68	AL2O3	12.39

1405	SIO2	45.40	MGO	23.31
1406	SIO2	43.84	FEO	13.83
1407	SIO2	43.20	AL2O3	22.69
1408	SIO2	51.24	MGO	21.21
1409	SIO2	51.02	FE2O3	13.05
1410	SIO2	45.27	MGO	13.05
1411	SIO2	44.66	AL2O3	14.49
1412	SIO2	44.66	AL2O3	14.35
1413	SIO2	44.20	AL2O3	13.93
1414	SIO2	43.97	AL2O3	14.10
1415	SIO2	51.01	FEO	17.62
1416	SIO2	43.61	MGO	16.53
1417	SIO2	52.01	MGO	15.16
1418	SIO2	41.85	MGO	16.24
1419	SIO2	39.62	FEO	17.74
1420	SIO2	36.22	FEO	26.42
1423	SIO2	40.60	MGO	18.30
1424	SIO2	43.00	MGO	20.60
1425	SIO2	41.10	MGO	17.90
1426	SIO2	49.58	MGO	14.00
1427	SIO2	53.81	MGO	18.24
1428	SIO2	45.12	FEO	15.23
1429	SIO2	44.78	FEO	14.94
1430	SIO2	40.96	FEO	16.88
1431	SIO2	42.80	FEO	14.61
1432	SIO2	42.78	FEO	14.15
1433	SIO2	42.36	AL2O3	17.66
1434	SIO2	50.44	MGO	15.87
1435	SIO2	45.36	FEO	12.79
1436	SIO2	40.04	FEO	15.23
1437	SIO2	52.90	FEO	28.00
1438	SIO2	39.63	AL2O3	14.36
1439	SIO2	41.90	MGO	15.10
1440	SIO2	40.00	MGO	14.60
1441	SIO2	40.00	AL2O3	13.60
1442	SIO2	40.60	AL2O3	14.20
1443	SIO2	40.60	AL2O3	13.70
1444	SIO2	40.60	FEO	13.90
1445	SIO2	55.63	MGO	19.13
1446	SIO2	51.88	MGO	18.48
1447	SIO2	52.78	MGO	17.43
1448	SIO2	34.69	FEO	14.67
1449	SIO2	45.50	MGO	13.05
1450	SIO2	45.37	MGO	18.94
1451	SIO2	42.54	MGO	12.64
1452	SIO2	44.35	MGO	16.36
1453	SIO2	38.82	FEO	25.87
1454	SIO2	37.69	AL2O3	13.41
1455	SIO2	60.04	MGO	24.00
1456	SIO2	50.02	FEO	14.09
1457	SIO2	46.40	FEO	17.38
1458	SIO2	47.34	MGO	13.89
1459	SIO2	51.86	MGO	19.40
1461	SIO2	54.58	MGO	20.43
1462	SIO2	52.19	MGO	20.00
1463	SIO2	50.37	FEO	40.08
1464	SIO2	40.71	FEO	24.39
1465	SIO2	44.56	MGO	15.50
1466	SIO2	44.07	MGO	14.20
1467	SIO2	40.96	FEO	13.30
1468	SIO2	44.36	FEO	16.63
1469	SIO2	43.20	MGO	13.27
1470	SIO2	55.90	MGO	15.68
1471	SIO2	55.60	MGO	16.70
1472	SIO2	55.00	MGO	19.92
1473	SIO2	53.50	MGO	14.50
1474	SIO2	55.00	MGO	16.10
1475	SIO2	52.80	MGO	16.30
1476	SIO2	55.00	MGO	17.30
1477	SIO2	55.00	MGO	19.70
1478	SIO2	55.80	FEO	12.53
1479	SIO2	43.15	AL2O3	14.06
1480	SIO2	43.10	MGO	14.02
1481	SIO2	37.51	FEO	23.21
1482	SIO2	38.81	FEO	21.72
1483	SIO2	52.59	FEO	11.80
1484	SIO2	50.62	FE2O3	12.40
1485	SIO2	50.00	FEO	12.46
1486	SIO2	47.21	AL2O3	13.48
1487	SIO2	38.81	FEO	21.72

1488	SIC2	37.51	FEO	23.21
1489	SIO2	43.71	AL2O3	14.98
1490	SIO2	46.11	MGO	17.00
1491	SIO2	45.12	MGO	14.83
1492	SIO2	46.45	MGO	16.55
1493	SIO2	43.08	MGO	14.17
1494	SIO2	42.50	MGO	14.30
1495	SIO2	50.10	MGO	16.80
1496	SIO2	49.00	MGO	15.90
1497	SIO2	46.30	MGO	15.00
1498	SIC2	48.90	MGO	17.30
1499	SIO2	51.00	FEO	21.90
1500	SIO2	51.00	FEO	27.00
1501	SIC2	53.00	FEO	18.00
1502	SIC2	55.00	MGO	18.00
1503	SIO2	55.00	FEO	16.10
1504	SIO2	52.00	MGO	15.00
1505	SIO2	55.00	FEO	18.00
1506	SIO2	52.00	FEO	20.00
1507	SIO2	55.00	MGO	20.50
1508	SIC2	55.00	MGO	17.50
1509	SIO2	54.00	MGO	15.50
1510	SIO2	56.00	MGO	22.00
1512	SIO2	58.00	MGO	22.00
1513	SIC2	56.00	MGO	21.00
1514	SIO2	55.00	MGO	22.00
1515	SIO2	51.00	MGO	22.50
1516	SIO2	52.00	MGO	21.00
1517	SIO2	49.00	MGO	21.00
1518	SIO2	51.00	MGO	21.00
1519	SIO2	54.00	MGO	21.50
1520	SIO2	55.00	MGO	20.00
1521	SIO2	52.00	MGO	21.00
1522	SIO2	55.00	K2O	22.00
1523	SIO2	56.00	K2O	22.00
1524	SIO2	52.00	K2O	21.00
1525	SIO2	53.00	K2O	23.00
1526	SIO2	49.00	FEO	34.70
1527	SIO2	50.00	FEO	36.70
1528	SIO2	49.00	FEO	41.20
1529	SIC2	50.00	FEO	38.60
1530	SIC2	48.00	FEO	38.60
1531	SIO2	50.00	FEO	34.70
1532	SIC2	54.00	FEO	38.60
1533	SIO2	53.00	FEO	36.70
1534	SIO2	51.00	FEO	40.50
1535	SIO2	50.00	FEO	35.40
1536	SIC2	51.00	FEO	34.10
1537	SIO2	51.00	FEO	28.30
1538	SIO2	48.00	FEO	37.30
1539	SIO2	54.00	FEO	25.70
1540	SIO2	53.00	FEO	24.40
1541	SIO2	55.00	FEO	22.50
1542	SIO2	54.00	FEO	32.20
1543	SIO2	54.00	FEO	27.00
1544	SIC2	48.00	FEO	20.00
1545	SIO2	51.00	FEO	34.10
1546	SIO2	48.00	FEO	46.30
1547	SIO2	50.00	FEO	45.60
1548	SIO2	52.00	FEO	45.60
1549	SIO2	49.00	FEO	43.80
1550	SIO2	54.00	FEO	25.70
1551	SIO2	46.00	FEO	28.30
1553	SIO2	48.48	FEO	42.05
1554	SIO2	40.10	FEO	27.58
1555	SIC2	40.53	MGO	16.81
1556	SIO2	43.86	MGO	13.85
1559	SIC2	42.30	AL2O3	15.68
1560	SIO2	39.86	FEO	14.71
1561	SIO2	39.02	MGO	17.62
1562	SIC2	38.98	MGO	14.88
1563	SIO2	53.06	MGO	13.21
1564	SIC2	46.89	FEO	12.08
1565	SIO2	40.29	MGO	13.51
1566	SIO2	43.23	MGO	11.68
1567	SIC2	44.31	MGO	16.22
1568	SIO2	40.44	AL2O3	15.61
1569	SIC2	39.73	AL2O3	13.75
1570	SIO2	45.91	AL2O3	18.25
1571	SIO2	43.41	AL2O3	19.04

1572	SIO2	51.26	MGO	16.14
1573	SIO2	46.56	CAO	14.25
1574	SIO2	48.50	FEO	20.10
1575	SIO2	47.40	FEO	24.60
1576	SIO2	46.90	FEO	25.60
1577	SIO2	49.00	FEO	13.63
1578	SIO2	48.80	FEO	35.10
1579	SIO2	47.60	FEO	34.90
1580	SIO2	53.50	FEO	32.80
1581	SIO2	55.01	MGO	23.85
1582	SIO2	45.71	AL2O3	12.98
1583	SIO2	53.46	AL2O3	11.76
1584	SIO2	57.64	AL2O3	14.75
1585	SIO2	56.00	AL2O3	13.46
1586	SIO2	49.04	AL2O3	16.28
1587	SIO2	46.14	FEO	13.28
1588	SIO2	42.66	FEO	22.24
1590	SIO2	42.09	MGO	14.78
1591	SIO2	41.61	AL2O3	12.16
1592	SIO2	46.30	MGO	12.66
1593	SIO2	43.98	FEO	12.59
1594	SIO2	43.65	MGO	13.96
1595	SIO2	48.40	MGO	15.86
1596	SIO2	50.87	FEO	22.90
1597	SIO2	46.55	MGO	21.68
1598	SIO2	38.10	FEO	25.56
1599	SIO2	56.16	MGO	21.37
1600	SIO2	52.91	MGO	16.51
1601	SIO2	52.54	MGO	17.12
1602	SIO2	46.38	MGO	16.20
1603	SIO2	41.27	AL2O3	13.62
1604	SIO2	41.26	FEO	18.70
1605	SIO2	39.37	FEO	20.81
1606	SIO2	44.77	FEO	14.70
1607	SIO2	43.54	FEO	12.89
1608	SIO2	42.94	FEO	13.68
1609	SIO2	41.44	AL2O3	13.82
1610	SIO2	40.92	AL2O3	14.10
1611	SIO2	42.17	MGO	14.46
1612	SIO2	44.54	FEO	17.82
1613	SIO2	41.73	FEO	14.00
1614	SIO2	41.25	FEO	15.94
1615	SIO2	45.87	MGO	21.79
1616	SIO2	43.99	AL2O3	15.04
1617	SIO2	41.67	FEO	16.18
1618	SIO2	42.55	FEO	12.02
1619	SIO2	42.45	AL2O3	14.29
1620	SIO2	37.41	FEO	23.24
1621	SIO2	45.34	MGO	13.01
1622	SIO2	46.54	MGO	17.81
1623	SIO2	46.22	MGO	14.53
1624	SIO2	46.01	MGO	13.96
1625	SIO2	44.05	MGO	14.86
1626	SIO2	43.90	MGO	15.81
1627	SIO2	43.78	FEO	12.57
1628	SIO2	42.73	FEO	13.88
1629	SIO2	45.83	MGO	14.89
1630	SIO2	44.02	MGO	13.96
1631	SIO2	43.24	MGO	12.96
1632	SIO2	42.06	AL2O3	14.54
1633	SIO2	41.57	AL2O3	13.47
1634	SIO2	40.76	AL2O3	14.50
1635	SIO2	47.48	MGO	20.09
1636	SIO2	42.05	AL2O3	12.69
1637	SIO2	41.89	AL2O3	12.70
1638	SIO2	41.71	AL2O3	13.93
1639	SIO2	41.56	FEO	13.78
1640	SIO2	41.54	FEO	14.34
1641	SIO2	41.23	AL2O3	13.56
1642	SIO2	48.88	MGO	12.56
1643	SIO2	47.42	FEO	15.98
1644	SIO2	44.87	FEO	13.30
1645	SIO2	43.01	FEO	17.61
1646	SIO2	45.76	MGO	14.08
1647	SIO2	39.83	AL2O3	16.03
1648	SIO2	49.37	FEO	19.31
1649	SIO2	44.16	FEO	14.23
1650	SIO2	37.36	FEO	21.62
1651	SIO2	49.05	MGO	11.45
1652	SIO2	55.48	AL2O3	14.64

1653	SIO2	60.45	MGO	12.12
1654	SIO2	47.33	MGO	21.38
1655	SIO2	37.30	FEO	19.66
1656	SIO2	38.73	FEO	15.57
1657	SIO2	47.81	FEO	15.10
1658	SIO2	45.33	AL2O3	15.55
1659	SIO2	44.21	AL2O3	15.11
1660	SIO2	44.51	FEO	15.28
1661	SIO2	44.49	FEO	13.62
1662	SIO2	42.99	FEO	14.03
1663	SIO2	43.47	AL2O3	15.33
1664	SIO2	42.15	AL2O3	15.64
1665	SIO2	47.34	MGO	13.64
1666	SIO2	41.10	FEO	14.16
1667	SIO2	39.50	AL2O3	14.29
1668	SIO2	39.77	MGO	15.02
1669	SIO2	43.90	MGO	13.48
1670	SIO2	50.36	MGO	14.82
1671	SIO2	41.90	MGO	18.54
1672	SIO2	46.40	MGO	21.96
1673	SIO2	54.32	MGO	21.16
1674	SIO2	54.84	MGO	15.28
1675	SIO2	56.04	MGO	22.20
1676	SIO2	55.10	MGO	22.04
1677	SIO2	56.60	MGO	22.26
1678	SIO2	56.00	MGO	22.12
1679	SIO2	57.30	MGO	25.20
1680	SIO2	56.10	MGO	24.94
1681	SIO2	51.94	FEO	19.39
1682	SIO2	50.71	FE2O3	20.45
1683	SIO2	50.66	FE2O3	22.64
1684	SIO2	47.35	FEO	36.60
1685	SIO2	47.04	FEO	26.10
1686	SIO2	50.00	FEO	40.50
1687	SIO2	50.81	FEO	33.88
1688	SIO2	51.64	FEO	34.38
1689	SIO2	52.11	FE2O3	20.62
1690	SIO2	51.89	FE2O3	19.22
1691	SIO2	52.13	FEO	21.25
1692	SIO2	51.03	FEO	21.19
1693	SIO2	38.92	FEO	14.64
1695	SIO2	42.60	AL2O3	13.65
1696	SIO2	40.26	AL2O3	13.23
1697	SIO2	56.43	MGO	22.86
1698	SIO2	41.99	FEO	14.32
1699	SIO2	57.47	MGO	24.87
1700	SIO2	57.61	MGO	24.12
1701	SIO2	57.43	MGO	24.83
1702	SIO2	57.78	MGO	24.12
1703	SIO2	56.13	MGO	21.18
1704	SIO2	56.36	MGO	21.20
1705	SIO2	54.85	MGO	20.24
1706	SIO2	54.75	MGO	20.36
1707	SIO2	57.07	MGO	19.35
1708	SIO2	51.64	MGO	19.61
1709	SIO2	52.58	MGO	19.12
1710	SIO2	52.05	MGO	19.42
1711	SIO2	43.92	MGO	12.67
1712	SIO2	43.60	MGO	12.60
1713	SIO2	41.92	FEO	14.28
1714	SIO2	42.06	FEO	14.36
1715	SIO2	36.86	FEO	23.35
1716	SIO2	39.41	AL2O3	12.71
1717	SIO2	39.55	AL2O3	13.27
1718	SIO2	39.88	AL2O3	17.49
1719	SIO2	40.02	AL2O3	17.68
1720	SIO2	45.79	MGO	21.11
1731	SIO2	36.16	FEO	15.11
1732	SIO2	36.04	FEO	16.52
1733	SIO2	36.02	FEO	16.50
1734	SIO2	34.51	FEO	18.28
1735	SIO2	37.10	FEO	14.13
1736	SIO2	37.94	FEO	13.13
1737	SIO2	50.23	FE2O3	18.34
1738	SIO2	47.78	FEO	12.76
1739	SIO2	50.26	MGO	13.40
1740	SIO2	37.44	FEO	13.44
1741	SIO2	42.05	CAO	14.25
1742	SIO2	38.95	FEO	12.04
1743	SIO2	37.61	CAO	13.92

1744	SIC2	51.35	FE2C3	18.31
1745	SIO2	49.30	FEO	22.35
1746	SIC2	41.55	FEO	21.30
1747	SIO2	4C.50	FEO	22.24
1748	SIO2	46.12	FEO	13.87
1749	SIC2	40.38	FEO	13.72
1750	SIO2	49.34	FEO	17.75
1751	SIO2	43.33	FEO	12.88
1752	SIO2	34.33	AL2C3	16.61
1753	SIO2	34.90	FEO	16.33
1754	SIO2	52.50	MGC	14.00
1755	SIO2	43.00	AL2C3	15.20
1756	SIC2	56.15	MGO	22.46
1760	SIO2	54.81	MGO	27.08
1761	SIC2	54.27	MGO	25.42
1762	SIO2	54.04	MGO	17.77
1763	SIO2	54.52	MGO	20.05
1764	SIO2	49.59	MGC	19.39
1765	SIO2	44.51	MGO	15.26
1766	SIO2	53.96	MGO	25.01
1767	SIO2	56.54	MGO	22.89
1768	SIO2	55.24	MGO	20.79
1769	SIO2	53.21	FEC	16.81
1770	SIO2	52.67	MGO	21.32
1771	SIC2	49.79	MGO	11.59
1772	SIC2	54.15	MGO	20.18
1773	SIO2	42.80	FEO	18.32
1774	SIO2	45.41	MGO	17.60
1775	SIO2	45.98	MGC	18.27
1776	SIO2	48.49	MGO	20.56
1777	SIO2	50.36	FEO	18.36
1778	SIC2	57.02	MGC	28.81
1779	SIO2	57.14	MGO	26.82
1780	SIO2	44.10	FEO	16.72
1781	SIO2	51.43	MGO	14.96
1782	SIO2	50.28	FEO	12.34
1783	SIO2	49.00	FEC	14.14
1784	SIO2	46.88	AL2O3	16.79
1785	SIO2	43.38	FEO	16.23
1786	SIC2	39.61	FEC	18.31
1787	SIC2	48.21	MGO	12.52
1788	SIO2	54.40	MGO	16.00
1789	SIO2	45.12	MGO	12.40
1790	SIO2	44.56	FEO	13.16
1791	SIO2	44.91	AL2O3	14.53
1792	SIO2	44.46	AL2O3	14.70
1793	SIC2	44.44	AL2O3	15.54
1794	SIO2	44.37	AL2C3	15.24
1795	SIC2	45.20	AL2O3	13.49
1796	SIC2	45.20	AL2O3	13.00
1797	SIC2	45.00	AL2C3	14.66
1798	SIO2	46.01	FEO	13.96
1799	SIC2	44.17	FEO	14.91
1800	SIC2	42.71	FEC	17.53
1801	SIO2	52.26	FEO	17.13
1802	SIO2	56.27	MGO	23.99
1803	SIO2	56.40	MGC	28.68
1804	SIO2	57.19	MGO	28.03
1805	SIC2	57.46	MGO	24.44
1806	SIO2	60.16	MGC	29.04
1807	SIC2	58.03	MGO	28.57
1808	SIO2	58.38	MGO	28.82
1809	SIC2	58.43	MGO	29.66
1810	SIC2	58.74	MGO	29.95
1811	SIO2	58.75	MGO	31.53
1812	SIO2	42.86	FEO	18.82
1813	SIC2	43.58	MGO	18.30
1814	SIO2	46.74	FEC	28.09
1815	SIO2	51.80	MGO	27.60
1816	SIC2	57.90	MGO	19.40
1817	SIO2	56.88	MGO	28.50
1818	SIC2	59.23	MGO	31.02
1819	SIO2	59.12	MGO	29.67
1820	SIO2	59.27	MGO	28.72
1821	SIC2	59.56	MGO	28.97
1822	SIO2	57.79	MGO	22.70
1823	SIC2	55.00	MGO	23.31
1824	SIC2	58.02	MGC	20.51
1825	SIO2	41.06	AL2O3	16.56
1826	SIC2	43.46	CAO	14.41

1827	SIO2	48.76	FEO	21.72
1828	SIO2	43.37	MGO	14.81
1829	SIO2	54.90	MGO	17.60
1830	SIO2	55.80	MGO	20.80
1831	SIO2	57.62	MGO	23.48
1832	SIO2	55.23	MGO	20.80
1833	SIO2	55.09	MGO	17.88
1834	SIO2	48.28	MGO	18.29
1835	SIO2	54.43	MGO	21.54
1836	SIO2	51.69	MGO	17.17
1837	SIO2	42.90	FEO	12.58
1838	SIO2	44.94	FEO	12.61
1839	SIO2	45.09	MGO	12.52
1840	SIO2	48.71	MGO	14.43
1841	SIO2	42.65	AL2O3	15.89
1842	SIO2	45.28	CAO	12.48
1843	SIO2	43.33	AL2O3	15.28
1844	SIO2	44.73	MGO	11.89
1845	SIO2	54.36	MGO	24.74
1846	SIO2	51.31	MGO	17.93
1847	SIO2	46.20	FEO	21.00
1848	SIO2	43.53	MGO	12.35
1849	SIO2	44.03	MGO	11.99
1850	SIO2	44.16	MGO	12.42
1851	SIO2	42.85	FEO	13.36
1852	SIO2	41.65	FEO	17.52
1853	SIO2	41.58	FEO	17.42
1854	SIO2	45.68	MGO	11.83
1855	SIO2	43.95	FEO	12.53
1856	SIO2	44.73	MGO	12.42
1857	SIO2	41.16	AL2O3	15.97
1858	SIO2	40.58	AL2O3	14.29
1859	SIO2	41.59	AL2O3	15.05
1860	SIO2	43.13	AL2O3	13.09
1861	SIO2	42.79	FEO	13.01
1862	SIO2	43.55	FEO	12.90
1863	SIO2	57.83	MGO	24.25
1864	SIO2	56.94	MGO	24.18
1865	SIO2	58.89	MGO	25.25
1866	SIO2	57.76	MGO	24.73
1867	SIO2	57.91	MGO	24.90
1868	SIO2	58.57	MGO	25.48
1869	SIO2	42.32	AL2O3	15.62
1870	SIO2	42.87	AL2O3	14.85
1871	SIO2	42.55	AL2O3	15.23
1872	SIO2	45.50	MGO	20.51
1873	SIO2	45.13	MGO	21.38
1874	SIO2	45.50	MGO	20.17
1875	SIO2	39.78	FEO	14.21
1876	SIO2	41.49	FEO	15.11
1877	SIO2	40.61	FEO	14.21
1878	SIO2	50.58	FEO	19.78
1879	SIO2	51.41	FEO	21.17
1880	SIO2	50.92	FEO	21.00
1881	SIO2	44.17	FEO	14.91
1882	SIO2	44.45	FEO	15.43
1883	SIO2	43.22	FEO	15.15
1884	SIO2	57.14	MGO	12.85
1885	SIO2	59.78	MGO	13.12
1886	SIO2	59.24	MGO	12.60
1887	SIO2	58.60	MGO	24.66
1888	SIO2	59.04	MGO	24.67
1889	SIO2	58.92	MGO	24.79
1890	SIO2	41.06	FEO	16.11
1891	SIO2	40.48	FEO	17.05
1892	SIO2	41.00	FEO	16.52
1893	SIO2	57.68	MGO	22.64
1894	SIO2	57.42	MGO	23.04
1895	SIO2	57.50	MGO	22.87
1896	SIO2	45.39	AL2O3	18.68
1897	SIO2	46.33	MGO	17.34
1898	SIO2	47.07	MGO	18.26
1899	SIO2	60.00	MGO	24.39
1900	SIO2	58.79	MGO	24.35
1901	SIO2	58.25	MGO	25.44
1902	SIO2	42.28	MGO	14.38
1903	SIO2	42.80	MGO	14.11
1904	SIO2	44.50	MGO	14.77
1905	SIO2	54.67	FEO	27.16
1906	SIO2	52.87	FEO	28.60

1907	SIO2	51.24	FEO	19.12
1908	SIO2	49.85	FEO	23.81
1909	SIO2	41.88	FEO	26.78
1910	SIO2	40.15	FEO	26.29
1911	SIO2	51.46	FEO	21.26
1912	SIO2	50.19	FEO	27.74
1913	SIO2	39.99	FEO	27.76
1914	SIO2	44.96	MGO	16.05
1915	SIO2	44.71	MGO	16.32
1916	SIO2	41.25	FEO	13.50
1917	SIO2	42.49	FEO	13.20
1918	SIO2	57.66	MGO	24.34
1919	SIO2	57.90	MGO	24.05
1920	SIO2	42.49	MGO	14.98
1921	SIO2	56.06	MGO	10.44
1922	SIO2	56.96	MGO	9.97
1923	SIO2	57.85	AL2O3	11.90
1924	SIO2	57.50	AL2O3	11.48
1925	SIO2	45.20	AL2O3	13.49
1926	SIO2	43.98	AL2O3	14.72
1927	SIO2	44.46	AL2O3	14.70
1928	SIO2	44.09	AL2O3	14.95
1929	SIO2	44.56	FEO	13.16
1930	SIO2	42.80	AL2O3	15.51
1931	SIO2	51.17	FEO	18.48
1932	SIO2	51.36	FEO	18.84
1933	SIO2	39.97	FEO	18.35
1934	SIO2	40.34	FEO	18.15
1935	SIO2	54.37	MGO	17.24
1936	SIO2	52.93	FEO	22.35
1937	SIO2	55.96	MGO	20.54
1938	SIO2	40.98	FEO	14.65
1939	SIO2	41.35	FEO	15.24
1940	SIO2	55.19	AL2O3	9.94
1941	SIO2	55.87	MGO	10.00
1942	SIO2	55.36	AL2O3	12.16
1943	SIO2	56.43	FEO	13.39
1944	SIO2	49.55	FEO	44.98
1945	SIO2	52.11	FEO	34.95
1946	SIO2	55.60	MGO	20.31
1947	SIO2	56.15	MGO	19.82
1948	SIO2	53.45	MGO	21.26
1949	SIO2	53.87	MGO	21.65
1950	SIO2	51.65	MGO	18.82
1951	SIO2	50.97	MGO	19.94
1952	SIO2	48.80	MGO	16.20
1953	SIO2	48.16	MGO	16.71
1954	SIO2	44.05	MGO	13.75
1955	SIO2	43.85	MGO	13.83
1956	SIO2	57.76	MGO	25.21
1957	SIO2	58.80	MGO	24.26
1958	SIO2	42.71	FEO	17.53
1959	SIO2	41.90	FEO	17.71
1960	SIO2	45.26	AL2O3	13.48
1961	SIO2	44.94	FEO	13.62
1962	SIO2	44.91	AL2O3	14.53
1963	SIO2	43.80	AL2O3	15.78
1964	SIO2	44.44	AL2O3	15.54
1965	SIO2	43.72	AL2O3	16.47
1966	FEO	45.83	SIO2	38.81
1967	SIO2	43.57	CAO	18.42
1968	SIO2	50.30	FEO	24.40
1969	SIO2	51.37	FE2O3	21.89
1970	SIO2	38.24	FEO	26.64
1971	SIO2	46.61	FEO	25.79
1972	SIO2	41.06	AL2O3	18.52
1973	SIO2	41.32	FEO	15.83
1974	SIO2	58.74	MGO	19.81
1975	SIO2	44.00	FEO	23.00
1976	SIO2	44.64	FEO	16.46
1977	SIO2	43.47	MGO	19.42
1978	SIO2	39.28	FEO	22.85
1979	SIO2	56.24	MGO	19.50
1980	SIO2	45.98	MGO	14.93
1981	SIO2	39.78	FEO	25.68
1982	SIO2	40.66	AL2O3	14.89
1983	SIO2	40.15	AL2O3	14.34
1984	SIO2	40.14	AL2O3	14.30
1985	SIO2	39.75	AL2O3	15.00
1986	SIO2	39.05	AL2O3	15.45

1987	SIO2	44.24	MGO	13.46
1988	SIO2	40.66	AL2O3	14.89
1989	SIO2	39.05	AL2O3	15.45
1990	SIO2	47.20	MGO	21.30
1991	SIO2	45.80	MGO	16.90
1992	SIO2	46.80	MGO	17.50
1993	SIO2	45.50	MGO	18.00
1994	SIO2	41.55	FEO	18.45
1995	SIO2	42.69	FEO	14.15
1996	SIO2	42.48	FEO	15.62
1997	SIO2	38.41	FEO	21.75
1998	SIO2	58.80	MGO	24.80
1999	SIO2	58.78	MGO	25.86
2000	SIO2	58.96	MGO	24.32
2001	SIO2	59.16	MGO	24.18
2002	SIO2	40.12	AL2O3	18.68
2003	SIO2	39.00	FEO	16.60
2004	SIO2	42.00	FEO	16.02
2005	SIO2	44.00	FEO	12.70
2006	SIO2	45.28	MGO	12.93
2007	SIO2	36.65	FEO	30.03
2008	SIO2	53.09	FE2O3	14.41
2009	SIO2	52.86	AL2O3	11.29
2010	SIO2	56.06	MGO	16.11
2011	SIO2	50.55	FEO	11.58
2012	SIO2	40.77	FEO	13.51
2013	SIO2	45.88	MGO	12.76
2014	SIO2	48.00	FEO	15.06
2015	SIO2	48.11	MGO	12.92
2016	SIO2	48.11	MGO	14.24
2017	SIO2	49.06	MGO	17.19
2018	SIO2	38.41	FEO	33.54
2024	SIO2	55.94	MGO	21.35
2025	SIO2	54.99	MGO	20.03
2026	SIO2	54.68	MGO	19.65
2027	SIO2	44.37	AL2O3	16.88
2028	SIO2	40.96	AL2O3	17.84
2029	SIO2	40.67	AL2O3	16.68
2030	SIO2	50.94	MGO	18.65
2031	SIO2	48.60	MGO	14.36
2032	SIO2	46.43	FEO	15.90
2033	SIO2	46.04	FEO	13.93
2034	SIO2	43.40	FEO	18.48
2035	SIO2	42.34	FEO	18.68
2036	SIO2	40.54	FEO	22.95
2037	SIO2	51.50	FEO	14.85
2038	SIO2	49.40	MGO	16.81
2039	SIO2	41.10	FEO	15.80
2040	SIO2	42.91	AL2O3	13.67
2041	SIO2	42.53	AL2O3	15.35
2042	SIO2	58.54	MGO	24.45
2043	SIO2	56.67	MGO	22.42
2044	SIO2	54.09	MGO	21.29
2045	SIO2	51.37	FEO	15.45
2046	SIO2	46.59	MGO	14.27
2047	SIO2	42.94	FEO	13.42
2048	SIO2	45.62	FEO	16.09
2049	SIO2	42.44	AL2O3	12.50
2050	SIO2	43.20	MGO	13.27
2051	SIO2	44.36	FEO	16.63
2252	SIO2	40.85	MGO	12.47
2053	SIO2	44.03	FEO	13.27
2054	SIO2	42.62	FEO	14.00
2055	SIO2	44.07	MGO	14.20
2056	SIO2	44.60	FEO	16.21
2057	SIO2	44.12	MGO	12.56
2058	SIO2	43.48	FEO	15.19
2059	SIO2	48.83	MGO	13.98
2060	SIO2	46.88	FEO	17.18
2061	SIO2	42.74	AL2O3	13.29
2062	SIO2	40.90	FEO	17.81
2063	SIO2	42.83	AL2O3	15.67
2064	SIO2	43.50	AL2O3	14.58
2065	SIO2	44.86	AL2O3	12.93
2066	SIO2	40.82	FEO	16.78
2067	SIO2	45.19	MGO	13.79
2068	SIO2	44.84	FEO	12.57
2069	SIO2	44.22	FEO	13.63
2070	SIO2	43.00	CAO	12.73
2071	SIO2	52.95	MGO	22.81

2072	SIO2	47.03	FEO	17.17
2073	SIO2	49.58	MGO	14.00
2074	SIO2	45.18	FEO	15.81
2075	SIO2	43.30	FEO	19.26
2076	SIO2	40.85	FEO	21.67
2077	SIO2	55.72	MGO	21.88
2078	SIO2	56.80	MGO	19.75
2079	SIO2	49.55	MGO	15.92
2080	SIO2	46.64	FEO	15.99
2081	SIO2	43.70	FEO	17.08
2082	SIO2	41.98	FEO	12.64
2083	SIO2	39.28	AL2O3	15.08
2084	SIO2	50.21	FEO	21.23
2085	SIO2	49.10	FEO	19.30
2086	SIO2	45.39	FEO	11.69
2087	SIO2	48.12	MGO	12.73
2088	SIO2	41.88	AL2O3	15.82
2089	SIO2	33.50	FEO	29.67
2090	SIO2	43.92	MGO	19.14
2091	SIO2	51.74	FEO	20.35
2092	SIO2	52.05	FEO	20.72
2093	SIO2	55.12	MGO	31.18
2094	SIO2	59.25	MGO	28.16
2095	SIO2	56.16	MGO	23.19
2096	SIO2	56.34	MGO	23.99
2097	SIO2	57.12	MGO	25.92
2098	SIO2	57.39	MGO	29.09
2099	SIO2	58.02	MGO	27.99
2100	SIO2	58.48	MGO	31.38
2101	SIO2	45.87	FEO	29.34
2102	SIO2	47.40	FEO	23.38
2103	SIO2	52.44	MGO	35.83
2104	SIO2	53.69	MGO	20.50
2105	SIO2	44.98	FEO	13.40
2106	SIO2	40.50	AL2O3	17.60
2107	SIO2	42.50	AL2O3	16.00
2108	SIO2	42.30	AL2O3	15.70
2109	SIO2	42.10	AL2O3	16.30
2110	SIO2	43.10	AL2O3	14.60
2111	SIO2	43.90	AL2O3	16.50
2112	SIO2	41.80	AL2O3	17.30
2113	SIO2	42.20	AL2O3	16.10
2114	SIO2	42.00	AL2O3	16.70
2115	SIO2	41.90	AL2O3	15.70
2116	SIO2	43.80	AL2O3	14.90
2117	SIO2	42.90	FEO	14.50
2118	SIO2	42.40	AL2O3	15.10
2119	SIO2	43.00	AL2O3	18.10
2121	SIO2	39.53	AL2O3	13.27
2128	SIO2	48.60	AL2O3	15.10
2129	SIO2	46.20	FEO	14.50
2130	SIO2	42.10	AL2O3	14.80
2131	SIO2	36.67	CAO	13.36
2132	SIO2	38.27	CAO	14.62
2133	SIO2	41.34	FEO	17.68
2134	SIO2	36.35	FEO	22.58
2135	SIO2	45.50	MGO	20.51
2136	SIO2	42.32	AL2O3	15.62
2137	SIO2	44.96	MGO	16.05
2138	SIO2	40.19	AL2O3	15.14
2139	SIO2	48.11	MGO	14.68
2140	SIO2	54.30	MGO	20.00
2141	SIO2	46.00	AL2O3	16.50
2142	SIO2	45.00	AL2O3	14.10
2143	SIO2	45.00	AL2O3	17.40
2144	SIO2	46.24	MGO	14.76
2145	SIO2	57.32	MGO	21.43
2146	SIO2	52.22	FEO	29.45
2147	SIO2	50.79	FEO	38.43
2150	SIO2	50.74	FEO	24.13
2151	SIO2	54.20	FEO	22.09
2152	SIO2	58.38	MGO	25.01
2153	SIO2	57.74	MGO	23.67
2154	SIO2	41.46	FEO	21.14
2155	SIO2	56.70	MGO	14.70
2156	SIO2	52.71	MGO	11.19
2157	SIO2	50.58	FE2O3	12.31
2158	SIO2	48.39	FE2O3	13.68
2159	SIO2	54.37	MGO	19.19
2160	SIO2	52.53	FE2O3	10.75

2161	SIO2	49.63	MGO	21.20
2162	SIO2	44.89	FEO	22.26
2163	SIO2	49.52	FE2O3	19.99
2164	SIO2	39.40	FE2O3	14.69
2165	SIO2	38.71	FE2O3	20.85
2166	SIO2	46.91	AL2O3	13.33
2167	SIO2	47.67	MGO	14.81
2168	SIO2	48.80	MGO	18.60
2169	SIO2	50.80	MGO	26.10
2170	SIO2	48.41	MGO	17.47
2171	SIO2	55.00	MGO	23.97
2172	SIO2	47.79	MGO	15.76
2173	SIO2	42.62	AL2O3	14.89
2174	SIO2	54.33	MGO	15.31
2175	SIO2	54.73	MGO	17.94
2176	SIO2	54.78	MGO	19.10
2177	SIO2	44.09	AL2O3	17.22
2178	SIO2	43.82	AL2O3	14.85
2179	SIO2	50.06	FEO	18.42
2180	SIO2	53.12	FEO	22.46
2182	SIO2	51.67	FEO	35.86
2183	SIO2	47.36	FEO	38.92
2184	SIO2	58.54	MGO	23.60
2185	SIO2	42.05	AL2O3	18.00
2186	SIO2	41.07	AL2O3	17.97
2187	SIO2	30.58	AL2O3	19.42
2188	SIO2	39.34	AL2O3	19.91
2189	SIO2	39.20	AL2O3	13.87
2190	SIO2	39.58	AL2O3	19.42
2191	SIO2	41.17	FEO	27.80
2192	SIO2	38.77	FEO	24.72
2193	SIO2	40.09	AL2O3	22.62
2194	SIO2	44.68	AL2O3	14.08
2195	SIO2	42.44	AL2O3	12.50
2196	SIO2	42.68	FEO	22.46
2197	SIO2	39.43	AL2O3	13.60
2198	SIO2	55.76	MGO	23.84
2199	SIO2	57.74	MGO	22.38
2200	SIO2	42.14	MGO	13.83
2201	SIO2	41.95	MGO	13.82
2202	SIO2	49.49	FEO	11.00
2203	SIO2	49.22	MGO	10.52
2204	SIO2	39.58	AL2O3	14.91
2205	SIO2	55.48	MGO	21.25
2206	SIO2	54.24	MGO	24.00
2207	SIO2	54.00	MGO	26.00
2208	SIO2	52.42	MGO	18.67
2209	SIO2	51.56	MGO	15.32
2210	SIO2	49.00	MGO	17.50
2211	SIO2	47.85	MGO	13.21
2212	SIO2	46.91	CAO	13.19
2213	SIO2	46.90	FE2O3	12.46
2214	SIO2	44.51	MGO	17.11
2215	SIO2	44.50	FEO	16.70
2216	SIO2	44.50	MGO	16.80
2217	SIO2	44.40	MGO	15.90
2218	SIO2	43.71	FEO	13.10
2219	SIO2	43.03	MGO	13.14
2220	SIO2	42.00	MGO	18.00
2221	SIO2	41.96	AL2O3	12.15
2222	SIO2	41.14	CAO	11.70
2223	SIO2	42.10	MGO	16.90
2224	SIO2	39.60	MGO	15.10
2225	SIO2	50.21	FEO	11.31
2226	SIO2	40.59	AL2O3	17.09
2227	SIO2	40.64	AL2O3	17.00
2228	SIO2	41.80	AL2O3	16.00
2229	SIO2	40.17	AL2O3	15.09
2230	SIO2	42.25	CAO	12.37
2231	SIO2	49.59	FEO	35.35
2232	SIO2	49.47	FEO	35.63
2233	SIO2	49.67	FEO	35.92
2234	SIO2	54.09	MGO	20.31
2235	SIO2	45.42	MGO	13.75
2236	SIO2	54.40	MGO	15.80
2237	SIO2	55.02	FE2O3	10.91
2238	SIO2	39.20	AL2O3	13.25
2239	SIO2	37.00	FEO	19.96
2240	SIO2	49.77	FEO	12.11
2241	SIO2	49.25	FEO	11.63

2242	SIO2	54.00	FE2O3	9.03
2243	SIO2	52.67	MGO	21.32
2244	SIO2	56.48	MGO	17.40
2246	SIO2	40.20	FEO	13.20
2247	SIO2	40.20	FEO	12.40
2248	SIO2	41.87	FEO	13.28
2249	SIO2	46.42	FEO	42.60
2250	SIO2	49.11	FEO	38.98
2252	SIO2	40.85	MGO	12.47
2253	SIO2	39.30	MGO	13.24
2254	SIO2	41.38	AL2O3	14.41
2255	SIO2	48.62	MGO	16.66
2256	SIO2	59.79	MGO	24.31
2257	SIO2	50.86	FEO	10.85
2258	SIO2	49.66	FEO	13.82
2259	SIO2	53.70	FEO	13.01
2260	SIO2	50.00	FEO	13.34
2262	SIO2	45.70	MGO	12.77
2263	SIO2	50.36	FEO	18.36
2264	SIO2	52.05	FEO	21.77
2265	SIO2	51.97	FEO	19.59
2266	SIO2	50.16	FEO	20.60
2267	SIO2	43.00	AL2O3	14.50
2268	SIO2	42.50	AL2O3	14.50
2269	SIO2	40.00	AL2O3	15.50
2270	SIO2	43.50	AL2O3	14.50
2271	SIO2	57.32	MGO	20.52
2272	SIO2	60.93	MGO	33.74
2273	SIO2	41.97	MGO	14.20
2274	SIO2	51.86	MGO	19.40
2275	SIO2	49.50	MGO	21.76
2276	SIO2	48.59	MGO	13.07
2277	SIO2	48.33	MGO	20.70
2278	SIO2	48.14	MGO	17.07
2279	SIO2	47.34	MGO	17.84
2280	SIO2	47.15	FEO	12.42
2281	SIO2	46.16	CAO	12.87
2282	SIO2	45.47	MGO	12.15
2283	SIO2	45.38	MGO	13.49
2284	SIO2	44.26	MGO	23.87
2285	SIO2	44.23	MGO	17.06
2286	SIO2	44.13	MGO	22.31
2287	SIO2	44.10	MGO	19.51
2288	SIO2	43.86	MGO	24.49
2289	SIO2	43.83	MGO	16.34
2290	SIO2	41.20	AL2O3	13.38
2291	SIO2	40.72	MGO	19.30
2292	SIO2	41.54	FEO	21.84
2293	SIO2	59.45	MGO	25.19
2294	SIO2	55.26	MGO	20.41
2295	SIO2	58.21	MGO	30.14
2296	SIO2	44.00	MGO	12.60
2297	SIO2	36.86	FEO	23.35
2298	SIO2	37.90	FEO	36.80
2299	SIO2	36.94	FEO	36.03
2300	SIO2	39.30	FEO	30.40
2301	SIO2	38.58	FEO	30.57
2302	SIO2	42.50	FEO	22.57
2303	SIO2	52.37	MGO	14.65
2304	SIO2	48.44	MGO	15.40
2305	SIO2	41.06	AL2O3	14.58
2306	SIO2	58.90	MGO	26.68
2307	SIO2	43.70	MGO	15.70
2308	SIO2	47.30	MGO	13.70
2309	SIO2	45.30	MGO	17.90
2310	SIO2	42.00	MGO	13.90
2311	SIO2	46.40	CAO	16.00
2312	SIO2	45.50	MGO	14.10
2313	SIO2	48.00	CAO	19.30
2314	SIO2	41.00	AL2O3	15.30
2315	SIO2	43.57	AL2O3	15.26
2316	SIO2	39.51	AL2O3	14.26
2318	SIO2	44.32	FEO	13.41
2319	SIO2	46.38	MGO	12.17
2321	SIO2	40.34	AL2O3	13.81
2322	SIO2	41.53	FEO	13.69
2324	SIO2	56.87	MGO	22.47
2325	SIO2	46.46	MGO	20.48
2326	SIO2	46.22	MGO	20.27
2327	SIO2	46.03	MGO	20.16

2328	SIO2	54.54	MGO	16.40
2329	SIO2	47.16	MGO	12.75
2336	SIO2	48.00	MGO	13.00
2337	SIO2	49.00	FE2O3	13.70
2338	SIO2	51.60	FEO	15.21
2339	SIO2	47.93	FEO	17.79
2340	SIO2	47.35	FEO	17.16
2341	SIO2	43.60	MGO	12.41
2342	SIO2	38.72	FEO	26.03
2343	SIO2	45.72	MGO	13.01
2344	SIO2	41.27	AL2O3	14.32
2345	SIO2	54.00	MGO	21.90
2346	SIO2	47.64	AL2O3	13.57
2347	SIO2	42.70	FEO	16.54
2348	SIO2	56.37	MGO	20.41
2349	SIO2	53.92	MGO	20.35
2350	SIO2	50.94	AL2O3	15.42
2351	SIO2	45.20	AL2O3	18.40
2352	SIO2	52.63	FEO	36.74
2353	SIO2	48.37	MGO	14.62
2354	SIO2	43.34	FEO	17.09
2355	SIO2	50.49	MGO	14.32
2356	SIO2	51.32	MGO	16.17
2357	SIO2	38.45	FEO	24.71
2358	SIO2	47.47	FEO	24.33
2359	SIO2	50.94	MGO	18.00
2360	SIO2	52.39	MGO	18.37
2361	SIO2	52.65	MGO	18.70
2362	SIO2	55.57	MGO	21.85
2363	SIO2	52.12	FE2O3	14.77
2364	SIO2	49.45	MGO	14.03
2365	SIO2	48.30	MGO	15.27
2366	SIO2	48.95	MGO	14.88
2367	SIO2	44.75	FEO	17.38
2368	SIO2	44.76	FEO	19.16
2369	SIO2	40.75	FEO	22.62
2370	SIO2	44.73	FEO	13.53
2371	SIO2	43.16	FEO	15.70
2372	SIO2	40.85	FEO	21.56
2373	SIO2	44.38	FEO	16.55
2374	SIO2	42.21	FEO	18.96
2375	SIO2	40.88	FEO	18.88
2376	SIO2	42.62	FEO	15.52
2377	SIO2	42.25	FEO	20.29
2378	SIO2	44.55	FEO	18.75
2379	SIO2	42.97	FEO	19.67
2380	SIO2	45.24	FEO	19.33
2381	SIO2	44.28	FEO	19.53
2382	SIO2	45.53	FEO	15.96
2383	SIO2	41.78	FEO	21.99
2384	SIO2	40.43	FEO	22.15
2385	SIO2	42.60	FEO	17.03
2386	SIO2	40.85	FEO	18.53
2387	SIO2	44.06	FEO	17.27
2388	SIO2	39.62	FEO	18.73
2389	SIO2	57.36	MGO	25.22
2390	SIO2	36.66	FEO	21.67
2391	SIO2	36.94	FEO	21.67
2392	SIO2	54.63	FEO	16.02
2393	SIO2	54.00	FEO	23.60
2394	SIO2	43.16	MGO	15.92
2395	SIO2	40.70	AL2O3	14.00
2396	SIO2	57.78	FEO	10.46
2397	SIO2	46.11	MGO	17.00
2398	SIO2	41.58	MGO	16.20
2399	SIO2	39.90	AL2O3	14.52
2400	SIO2	40.92	AL2O3	15.05
2401	SIO2	41.00	MGO	17.90
2402	SIO2	40.12	MGO	14.48
2403	SIO2	40.34	MGO	13.70
2404	SIO2	40.22	AL2O3	14.45
2405	SIO2	39.50	MGO	12.90
2406	SIO2	40.00	AL2O3	12.90
2407	SIO2	38.30	AL2O3	14.80
2408	SIO2	40.80	MGO	12.00
2409	SIO2	41.30	FEO	14.50
2410	SIO2	40.10	FEO	14.20
2411	SIO2	38.50	FEO	14.90
2412	SIO2	39.20	FEO	14.60
2413	SIO2	39.80	FEO	16.20

2414	SIO2	40.00	FEO	18.90
2415	SIO2	38.80	FEO	22.80
2416	SIO2	38.60	FEO	23.80
2417	SIO2	39.30	FEO	23.50
2418	SIO2	47.80	FEO	33.30
2419	SIO2	54.52	MGO	25.11
2420	SIO2	44.59	MGO	19.50
2421	SIO2	43.37	MGO	16.89
2422	SIO2	51.84	FEO	24.72
2423	SIO2	50.22	FEO	41.28
2424	SIO2	58.99	MGO	24.74
2425	SIO2	42.05	MGO	14.90
2426	SIO2	42.25	CAO	13.98
2427	SIO2	41.15	AL2O3	16.14
2428	SIO2	41.67	FEO	14.92
2429	SIO2	41.40	FEO	13.61
2430	SIO2	45.90	MGO	16.38
2431	SIO2	45.84	MGO	12.86
2432	SIO2	43.58	MGO	13.96
2433	SIO2	50.42	MGO	16.17
2434	SIO2	43.84	CAO	19.94
2435	SIO2	40.96	MGO	17.37
2436	SIO2	40.96	AL2O3	17.84
2437	SIO2	44.37	AL2O3	16.88
2438	SIO2	43.86	AL2O3	14.20
2439	SIO2	40.12	AL2O3	12.83
2440	SIO2	38.48	AL2O3	14.46
2441	SIO2	43.21	MGO	14.32
2442	SIO2	40.37	AL2O3	13.35
2443	SIO2	43.50	MGO	12.52
2444	SIO2	50.94	MGO	18.65
2445	SIO2	53.20	MGO	20.53
2446	SIO2	56.08	MGO	23.05
2447	SIO2	57.54	MGO	24.78
2448	SIO2	54.84	MGO	15.30
2449	SIO2	53.06	MGO	15.67
2450	SIO2	52.40	MGO	15.67
2451	SIO2	55.74	MGO	22.15
2452	SIO2	55.52	MGO	21.67
2453	SIO2	55.28	MGO	20.89
2454	SIO2	38.26	AL2O3	15.50
2455	SIO2	54.12	MGO	17.88
2456	SIO2	44.60	FEO	19.91
2457	SIO2	44.50	FEO	21.83
2458	SIO2	42.75	FEO	17.67
2459	SIO2	47.05	FEO	19.23
2460	SIO2	50.25	FE2O3	17.22
2461	SIO2	53.40	FE2O3	15.68
2462	SIO2	49.25	FEO	18.76
2463	SIO2	48.22	FEO	23.74
2464	SIO2	52.97	FEO	15.70
2465	SIO2	45.85	FE2O3	13.66
2466	SIO2	47.76	FEO	25.66
2467	SIO2	48.75	FEO	20.68
2468	SIO2	50.90	FEO	16.85
2469	SIO2	47.12	FEO	18.09
2470	SIO2	48.85	FEO	18.76
2471	SIO2	50.23	FE2O3	18.34
2472	SIO2	49.34	FEO	17.75
2473	SIO2	43.04	FE2O3	21.01
2474	SIO2	43.46	FE2O3	19.57
2475	SIO2	50.34	FE2O3	19.27
2476	SIO2	46.82	FEO	20.29
2477	SIO2	48.27	FEO	21.83
2478	SIO2	47.76	FEO	19.91
2479	SIO2	47.81	FEO	21.83
2480	SIO2	47.86	FEO	19.91
2481	SIO2	48.24	FEO	20.29
2482	SIO2	47.20	FE2O3	22.33
2483	SIO2	46.20	FE2O3	21.66
2484	SIO2	47.56	FEO	19.77
2485	SIO2	47.72	FE2O3	19.07
2486	SIO2	48.40	FEO	18.48
2487	SIO2	48.02	FE2O3	19.65
2488	SIO2	46.20	FE2O3	21.66
2489	SIO2	47.44	FEO	18.82
2490	SIO2	48.22	FEO	19.69
2491	SIO2	48.76	FE2O3	19.39
2492	SIO2	47.78	FEO	12.76
2495	SIO2	57.66	MGO	24.34

2496	SIO2	56.10	FE2O3	15.60
2498	SIO2	59.44	AL2O3	12.78
2499	SIO2	48.75	MGO	12.78
2500	SIO2	58.04	MGO	11.71
2504	SIO2	54.00	FEO	20.00
2507	SIO2	51.00	FEO	34.10
2508	SIO2	51.19	FEO	21.27
2514	SIO2	52.16	FEO	18.19
2516	SIO2	56.00	MGO	20.00
2518	SIO2	52.60	MGO	17.95
2522	SIO2	60.60	MGO	33.40
2525	SIO2	38.03	FEO	18.19
2531	SIO2	47.68	MGO	20.68
2532	SIO2	47.86	MGO	19.89
2533	SIO2	44.72	MGO	16.69
2534	SIO2	40.75	AL2O3	19.81
2541	SIO2	51.00	MGO	21.17
2542	SIO2	51.12	MGO	18.54
2543	SIO2	53.02	FEO	24.40
2544	SIO2	52.09	FEO	26.02
2545	SIO2	53.54	FEO	23.12
2546	SIO2	44.75	MGO	14.24
2547	SIO2	44.78	AL2O3	13.33
2548	SIO2	42.53	FEO	14.99
2549	SIO2	44.64	FEO	17.25
2550	SIO2	51.40	FEO	26.30
2551	SIO2	52.20	FEO	26.80
2554	SIO2	58.31	MGO	27.17
2555	SIO2	51.27	FEO	31.74
2556	SIO2	55.80	MGO	21.00
2557	SIO2	56.49	MGO	24.57
2558	SIO2	56.16	MGO	19.84
2559	SIO2	52.28	FEO	22.57
2560	SIO2	55.50	MGO	21.49
2561	SIO2	55.53	MGO	19.05
2562	SIO2	55.70	MGO	17.00
2563	SIO2	55.24	MGO	14.04
2564	SIO2	54.70	MGO	16.70
2565	SIO2	55.70	MGO	17.00
2566	SIO2	52.80	FEO	22.50
2567	SIO2	52.60	FEO	22.20
2568	SIO2	47.50	FEO	14.80
2569	SIO2	48.90	FEO	16.10
2570	SIO2	54.00	FEO	18.20
2571	SIO2	54.28	MGO	10.05
2572	SIO2	54.36	FE2O3	11.03
2573	SIO2	53.20	FEO	15.30
2574	SIO2	54.80	FEO	16.70
2575	SIO2	52.70	FEO	20.00
2576	SIO2	54.40	MGO	14.50
2577	SIO2	53.10	FEO	14.60
2578	SIO2	51.30	MGO	15.60
2579	SIO2	53.33	FEO	15.90
2580	SIO2	47.50	MGO	12.74
2581	SIO2	53.04	FEO	19.44
2582	SIO2	53.46	MGO	13.80
2587	SIO2	56.76	MGO	24.15
2588	SIO2	41.60	MGO	15.50
2589	SIO2	42.50	FEO	22.00
2590	SIO2	52.40	FEO	16.75
2591	SIO2	52.40	FEO	16.90
2592	SIO2	54.70	FEO	20.40
2593	SIO2	44.08	MGO	12.55
2594	SIO2	41.96	FEO	18.78
2595	SIO2	44.96	FEO	16.28
2596	SIO2	43.98	FEO	16.45
2597	SIO2	45.45	FEO	16.75
2598	SIO2	53.12	FEO	24.72
2599	SIO2	48.00	FEO	14.68
2600	SIO2	47.70	FEO	14.07
2601	SIO2	47.40	MGO	16.10
2602	SIO2	50.30	MGO	16.90
2603	SIO2	38.70	FEO	22.70
2604	SIO2	40.30	FEO	17.40
2605	SIO2	39.50	FEO	18.80
2606	SIO2	41.30	FEO	15.90
2607	SIO2	52.50	FEO	27.30
2608	SIO2	52.70	FEO	26.20
2609	SIO2	53.60	FEO	22.50
2610	SIO2	53.90	FEO	22.60

2611	SIO2	53.70	FEO	21.60
2612	SIO2	53.50	FEO	22.00
2613	SIO2	53.50	FEO	20.90
2614	SIO2	53.70	FEO	21.40
2615	SIO2	53.60	FEO	20.60
2616	SIO2	54.50	FEO	20.30
2617	SIO2	53.20	FEO	19.50
2618	SIO2	53.40	MGO	19.90
2619	SIO2	54.20	MGO	19.60
2620	SIO2	54.00	MGO	19.90
2621	SIO2	54.90	MGO	20.70
2622	SIO2	51.00	FEO	22.30
2623	SIO2	50.60	FEO	21.60
2624	SIO2	52.40	FEO	21.70
2625	SIO2	51.00	FEO	20.80
2626	SIO2	52.40	FEO	21.40
2627	SIO2	52.50	FEO	20.40
2628	SIO2	52.90	MGO	19.60
2629	SIO2	53.60	MGO	19.70
2630	SIO2	53.70	MGO	20.20
2631	SIO2	54.10	MGO	21.30
2632	SIO2	53.50	MGO	22.60
2633	SIO2	55.70	MGO	23.70
2634	SIO2	55.80	MGO	24.10
2635	SIO2	57.10	MGO	28.20
2636	SIO2	56.80	MGO	28.40
2637	SIO2	41.20	FEO	25.80
2638	SIO2	40.80	FEO	25.00
2639	SIO2	41.20	FEO	24.30
2640	SIO2	40.70	FEO	24.10
2641	SIO2	46.00	FEO	22.30
2642	SIO2	45.00	FEO	21.80
2643	SIO2	44.30	FEO	21.80
2644	SIO2	47.30	FEO	19.50
2645	SIO2	47.10	MGO	18.50
2646	SIO2	42.80	FEO	20.00
2647	SIO2	42.90	FEO	19.70
2648	SIO2	43.20	FEO	15.80
2649	SIO2	44.80	AL2O3	14.60
2650	SIO2	45.30	FEO	14.00
2651	SIO2	44.70	AL2O3	14.20
2652	SIO2	44.30	AL2O3	16.20
2653	SIO2	44.00	AL2O3	15.00
2654	SIO2	44.90	AL2O3	14.60
2655	SIO2	45.40	MGO	13.80
2656	SIO2	47.30	MGO	15.30
2657	SIO2	45.40	MGO	16.30
2658	SIO2	55.50	MGO	22.80
2659	SIO2	56.40	MGO	23.10
2661	SIO2	42.60	FEO	14.30
2662	SIO2	40.60	AL2O3	14.50
2663	SIO2	41.70	FEO	13.20
2664	SIO2	43.30	MGO	13.20
2665	SIO2	42.96	FEO	14.21
2666	SIO2	46.95	FEO	16.77
2667	SIO2	48.12	FEO	16.58
2668	SIO2	40.70	FEO	13.60
2669	SIO2	45.00	MGO	16.10
2670	SIO2	49.70	MGO	27.60
2671	SIO2	47.10	MGO	20.00
2672	SIO2	42.50	MGO	18.30
2673	SIO2	35.80	FEO	32.30
2674	SIO2	45.50	FEO	27.70
2675	SIO2	42.95	FEO	16.79
2676	SIO2	42.56	FEO	17.37
2677	SIO2	42.01	FEO	17.22
2678	SIO2	41.47	AL2O3	18.14
2679	SIO2	42.46	FEO	17.42
2680	SIO2	42.49	FEO	17.34
2681	SIO2	45.14	FEO	14.66
2682	SIO2	43.44	AL2O3	15.33
2683	SIO2	46.70	FEO	14.45
2684	SIO2	45.22	FEO	14.89
2685	SIO2	42.44	FEO	17.20
2686	SIO2	41.42	FEO	20.63
2687	SIO2	42.60	AL2O3	15.60
2688	SIO2	43.35	FEO	17.49
2689	SIO2	41.48	FEO	19.18
2690	SIO2	57.70	MGO	23.50
2691	SIO2	58.00	MGO	23.80

2692	SIO2	58.30	MGO	23.80
2693	SIO2	57.80	MGO	23.90
2694	SIO2	58.30	MGO	24.20
2695	SIO2	57.60	MGO	23.60
2696	SIO2	57.50	MGO	23.80
2697	SIO2	57.70	MGO	23.60
2698	SIO2	56.80	MGO	23.10
2699	SIO2	57.60	MGO	23.90
2700	SIO2	58.40	MGO	24.10
2701	SIO2	58.20	MGO	32.00
2702	SIO2	58.30	MGO	31.60
2703	SIO2	58.40	MGO	31.90
2704	SIO2	51.07	FEO	36.82
2705	SIO2	49.79	FEO	20.49
2706	SIO2	45.83	MGO	13.38
2707	SIO2	44.89	FEO	12.42
2708	SIO2	41.10	AL2O3	16.00
2709	SIO2	41.90	AL2O3	15.50
2710	SIO2	41.40	AL2O3	15.90
2711	SIO2	40.60	MGO	13.80
2712	SIO2	41.70	MGO	14.10
2713	SIO2	42.20	MGO	13.50
2714	SIO2	45.20	MGO	14.60
2715	SIO2	41.00	MGO	14.00
2716	SIO2	42.10	FEO	13.80
2717	SIO2	37.40	AL2O3	15.70
2718	SIO2	37.60	MGO	13.60
2719	SIO2	40.10	FEO	21.50
2720	SIO2	40.00	AL2O3	15.30
2721	SIO2	40.00	AL2O3	14.60
2722	SIO2	40.50	AL2O3	15.30
2723	SIO2	40.00	AL2O3	14.50
2724	SIO2	40.20	AL2O3	14.40
2725	SIO2	40.20	AL2O3	15.00
2726	SIO2	40.20	MGO	15.10
2727	SIO2	43.20	MGO	15.80
2728	SIO2	54.28	MGO	12.38
2729	SIO2	55.06	MGO	13.51
2730	SIO2	54.40	MGO	15.83
2731	SIO2	53.95	MGO	15.66
2732	SIO2	54.25	MGO	14.57
2733	SIO2	54.60	MGO	14.63
2734	SIO2	54.58	MGO	15.67
2735	SIO2	53.78	MGO	14.64
2736	SIO2	54.82	MGO	16.14
2737	SIO2	45.00	FE2O3	22.30
2738	SIO2	43.80	FE2O3	20.00
2739	SIO2	41.34	FEO	17.68
2740	SIO2	36.35	FEO	22.58
2741	SIO2	42.96	CAO	14.11
2742	SIO2	43.38	CAO	13.91
2743	SIO2	41.92	FEO	13.58
2744	SIO2	41.68	FEO	13.62
2745	SIO2	36.34	FEO	22.99
2746	SIO2	40.26	AL2O3	14.12
2747	SIO2	45.12	FEO	16.96
2748	SIO2	45.72	FEO	15.52
2749	SIO2	44.46	FEO	16.36
2750	SIO2	46.14	FEO	14.37
2751	SIO2	46.12	MGO	13.95
2752	SIO2	43.64	MGO	12.28
2753	SIO2	44.48	FEO	17.70
2754	SIO2	41.97	FEO	21.77
2755	SIO2	41.96	MGO	11.59
2756	SIO2	47.17	MGO	13.27
2757	SIO2	46.87	MGO	13.68
2758	SIO2	48.63	MGO	14.11
2759	SIO2	48.11	MGO	14.43
2760	SIO2	39.72	AL2O3	14.26
2761	SIO2	38.79	AL2O3	14.35
2762	SIO2	37.77	FEO	20.89
2763	SIO2	40.00	AL2O3	16.00
2764	SIO2	40.00	AL2O3	16.00
2766	SIO2	40.00	AL2O3	16.00
2767	SIO2	38.45	FEO	25.15
2768	SIO2	38.85	FEO	21.05
2769	SIO2	39.62	FEO	18.25
2770	SIO2	45.69	FEO	22.38
2771	SIO2	50.05	FEO	26.35
2772	SIO2	56.06	MGO	21.88

2788	SIO2	57.80	MGO	22.40
2789	SIO2	54.90	FEO	12.10
2790	SIO2	56.56	AL2O3	12.27
2791	SIO2	50.03	CAO	12.51
2792	SIO2	48.85	MGO	13.51
2793	SIO2	52.13	MGO	17.21
2794	SIO2	52.96	MGO	17.41
2795	SIO2	48.11	MGO	13.35
2796	SIO2	44.36	FEO	14.50
2797	SIO2	44.95	FEO	13.60
2798	SIO2	51.39	MGO	16.81
2799	SIO2	45.54	MGO	12.76
2800	SIO2	46.59	MGO	14.27
2801	SIO2	42.89	AL2O3	13.95
2805	SIO2	44.81	MGO	16.45
2806	SIO2	44.51	AL2O3	17.10
2807	SIO2	42.47	AL2O3	17.81
2808	SIO2	42.70	AL2O3	18.26
2809	SIO2	43.50	AL2O3	17.90
2810	SIO2	53.80	MGO	19.45
2811	SIO2	50.01	MGO	20.99
2812	SIO2	52.97	MGO	13.44
2813	SIO2	45.15	MGO	13.92
2814	SIO2	45.92	MGO	15.34
2815	SIO2	46.65	MGO	13.26
2816	SIO2	56.80	MGO	11.85
2817	SIO2	56.13	MGO	17.61
2818	SIO2	55.29	FEO	15.67
2819	SIO2	52.58	FEO	16.57
2820	SIO2	49.54	FEO	18.55
2823	SIO2	52.99	FEO	18.27
2824	SIO2	49.90	FEO	16.20
2822	SIO2	53.61	FEO	18.35
2825	SIO2	54.40	FEO	16.00
2826	SIO2	49.70	MGO	13.90
2827	SIO2	55.50	FEO	12.60
2828	SIO2	48.60	FEO	14.40
2829	SIO2	55.80	FEO	12.40
2830	SIO2	48.10	MGO	13.20
2831	SIO2	55.30	FEO	13.10
2832	SIO2	52.28	MGO	18.14
2833	SIO2	43.30	MGO	16.02
2834	SIO2	41.43	MGO	14.48
2835	SIO2	40.13	MGO	14.27
2836	SIO2	37.57	AL2O3	14.91
2837	SIO2	50.78	FEO	29.64
2838	SIO2	42.05	FEO	19.36
2839	SIO2	53.02	FEO	22.19
2840	SIO2	54.20	MGO	20.90
2841	SIO2	54.50	MGO	21.40
2842	SIO2	54.10	MGO	21.20
2843	SIO2	49.38	FEO	19.17
2844	SIO2	53.00	MGO	10.72
2845	SIO2	52.58	MGO	16.57
2846	SIO2	54.74	MGO	15.49
2847	SIO2	46.47	FEO	14.98
2849	SIO2	45.41	FEO	17.38
2850	SIO2	49.61	MGO	15.14
2851	SIO2	44.38	FEO	16.72
2852	SIO2	49.31	FEO	10.68
2853	SIO2	47.23	FEO	15.61

APPENDIX 9.

CONVENTIONS USED IN TRANSCRIBING THE DATA IN THE AMPHIBOLE DATA FILE.

The aim of this Appendix is to describe how information has been transcribed so that further users can maintain uniformity in data extension and at the same time reduce possible misunderstandings when asking queries of the data file. A complete list of relation and domain names is given in Appendix 7.

1. Relation REFERENCE.

REFERENCE (REF. NO., AUTHOR , AUTHORINITIALS , ANALYST , ANALYSTINITIALS , DATE , REFERENCE , VOLUME)

Contains information relating to the original literature reference from which the amphibole analysis was obtained. Normally all the relevant information can be contained in one tuple. If there is more than one author responsible for an article a tuple is formed for each of the authors in turn as if each was the sole author. The same REF.NO. is used for each tuple concerned. In this way it is possible to query the data base for an author and obtain information of all those references in which he is senior or joint author. There is no way of identifying the senior author.

1.1. AUTHOR.

The authors surname.

Conventions.

Because of a Pl/1 character string restriction apostrophes in surnames have been removed, O'Hare becomes OHARE. Spaces in names such as VAN DER PLAS are maintained as single blanks.

1.2. AUTHORINITIALS.

The author's initials.

Conventions.

Each initial is followed by a full stop. Abbreviations such as 'JR.' have been included.

1.3. ANALYST

The surname of the analyst.

Convention.

As 1.1.

1.4. ANALYSTINITIALS.

The analyst's initials.

Conventions.

As 1.2.

1.5. DATE.

The year of publication of the reference.

Convention.

No difference is made between several articles written by the same author in one year.

1.6. REFERENCE.

The title of the journal or book from which the data was taken.

Convention.

Journals are quoted in their standard abbreviated form. Each abbreviated word is followed by a full stop and if appropriate a blank. Non-abbreviated words are separated by a blank. The complete field was left blank if the data was taken from a secondary source. When the original source has been consulted this domain is completed. The original source can be also found with the help of Appendix 8.

1.7. VOLUME.

The volume and page numbers of the article is entered here. In addition for those references in which there is more than a single author the surhames of the additional joint authors are included.

Conventions.

The volume number is abbreviated to 'V.' and the page

numbers as 'P.') followed without intervening blanks by the number. In those cases in which there is more than one author, the page and volume numbers are followed by an intervening blank and the word 'WITH' (abbreviated to 'W'), an intervening blank, and then the authors initials and surname. References with four or more authors have been denoted by the form 'WITH OTHERS'.

2. Relation ANALYSIS.

ANALYSIS (REF.NO. , REF.CODE.)

Contains the code number or character string used by the author to identify an analysis.

Convention.

Identification codes containing gaps of undefined length have been encoded as single blanks.

3. Relation MINERALNAME.

MINERALNAME (REF.NO. , NAME)

Contains the name used by the author for the mineral. The term 'amphibole' has been considered a valid response.

Convention.

English spelling has been used throughout, provided there is no ambiguity.

4. Relation GEOGRAPHY.

GEOGRAPHY (REF.NO. , COUNTRY , COUNTY , LOCALITY)

Geographical information has been entered under three domains. Unfortunately this representation sadly underates the information present in many cases. For example, all combinations of geo-political, physiographic, geographic divisions are possible both in the literature source and as possible retrieval criteria. Despite this disadvantage, information described in terms of three domains is sufficient for most queries.

4.1. COUNTRY.

The name of the country.

Convention.

The English spelling for the country has been used. Abbreviations were restricted to 'U.S.A.' and 'U.S.S.R.' Where the name or boundaries of a country have changed with time the name in the original source has been used.

4.2. COUNTY.

Contains a large scale geographic or physiographic subdivision of the country of origin. This includes such regions as 'states', 'counties', 'provinces', 'areas', 'perfectures', 'mountains' etc.

Conventions.

The names of the regions are entered without being followed by their status except in the case of Japanese 'perfectures' (abbreviated to 'PERFECT') or physiographic regions.

4.3. LOCALITY.

The exact locality from which the amphibole was collected.

Conventions.

None.

5. Relation OCCURRENCE.

OCCURRENCE (REF.NO. , ROCKNAME)

Contains the rocktype in which the amphibole was found.

Conventions.

No attempt was made to systmatise the responses or to apply any classification. Materials which have been synthesised are encoded as 'SYNTHETIC' and those which have been heated are encoded as 'HEATED'.

6. Relation OPTICS.

OPTICS (REF.NO. , ALPHA , ALPHAERROR , BETA , BETAERROR,

GAMMA , GAMMAERROR , 2V , DISPERSION , ORIENTATION , O.A.P. , DELTA , DELTAERROR , EXT. L.)

Contains the optical properties of amphiboles determined either in sodium or white light.

Conventions.

All Greek letters are encoded as their word equivalences. The symbol '$\wedge$', meaning an angle, has been replaced by ':'.

6.1. ALPHA , BETA , GAMMA.

The refractive indices for the three principal refractive indices.

Convention.

The refractive index is quoted to the number of decimal places used by the author. During transcription the following equivalences of (Bloss 1966, p. 151) have been recognised.

α = N = Np = Nx = nX = X = Na = Nx = N1

β = N = Nm = Ny = nY = Y = Nb = Ny = N2

γ = N = Ng = Nz = nZ = Z = Nc = Nz = N3

6.2. ALPHAERROR , BETAERROR , GAMMAERROR.

Contains the error in determination of the refractive indices.

Convention.

Where an error is quoted in the form $\pm$ 0.001, this is encoded as 0.001.

6.2. 2V.

Contains the sign and value of the optic axial angle. Surprisingly often both pieces of information are not given.

Convention.

2V is entered as the value of the optic axial angle preceeded by its sign. If the optic axial angle is given in terms of a

principal refractive index the following equivalences are recognised.

$2V_\alpha = 2Vx = -ve,$

$2V_\gamma = 2Vz = +ve.$

Because it is possible to describe the optic axial angle relative to one principal refractive index irrespective of sign the following coding sequence has been followed :-

a) if the sign and value are given enter directly.

b) If the 2V and direction in terms of principal refractive index, enter the sign as appropriate to the refractive index, e.g. $2V_\alpha = 40 = -40$, $2V_\alpha = 100 = -100$ not +80.

c) if no sign is given then default the sign to negative. The validity of this can then be checked on data validification, see Section 4.4.

d) if only the sign is given then no entry is made.

Where explicitly stated 2V is entered in preference to 2E.

6.4. DISPERSION.

Convention.

Valid responses are of the type 'V=R','V> R', 'R<V' or 'NONE', where R stands for red and V for violet.

Optical Orientation., including domains O.A.P. , EXT. L. , ORIENTATION.

To comply with the habit of describing the orientation of the principal refractive indices with respect to the crystallographic axes in terms of (i) the orientation of the optic axial plane, (ii) the extinction angle between a refractive index and a crystallographic axis, and (iii) the parallelism of principal refractive indices and crystallographic axes, three domains O.A.P., EXT. L., and ORIENTATION have been used. It should be noted that in some instances there exists more than one unique method of defining the orientation of the

indicatrix. Thus for an orthorhombic amphibole X = α Y = β defines the same orientation as Z = γ, O.A.P. = 010. All three domains should be considered together.

6.6. ORIENTATION.

The parallelism of principal refractive indices and crystallographic axes is included here.

Convention.

Coded in the manner used by the author.

6.7. O.A.P.

The direction of the optic axial plane.

Convention.

A response given solely in terms of the Millers indices for a plane '010' signifies that the O.A.P. lies parallel to the (010) plane. If the O.A.P. is given as perpendicular to a direction it is coded as 'PERP 010'.

6.9. DELTA , DELTAERROR.

Contains the birefringence and its error of determination.

Conventions.

As 6.1, 6.2.

6.9. EXTINCTION

Contains the extinction angle between a stated principal refractive index and a crystallographic axis.

Conventions.

The authors form is used except that the symbol for an angle '$\wedge$' is replaced by ':'.

7. Relation PLEOCHROISM.

PLEOCHROISM (REF.NO., FORMULA, X, Y, Z)

Under this heading are grouped the optical effects produced by absorption. For most amphiboles the angle between the principal directions of the indicatrix and the three absorption axes X, Y and Z,

is small and can be neglected. Unless explicitly stated to the contrary it has been assumed that the X, Y, Z, and α , β ,γ pleochroic schemes are synonomous. If it is explicitly stated to the contrary that the axes are not parallel the values for X, Y, Z, have been used.

7.1. FORMULA.

The absorption formula where explicitly stated.

Conventions.

The formula is written in terms of the axes X, Y, Z each separated by one of the comparisons '<', '=', '>'

7.2. X, Y, Z.

The pleochroic scheme along the three principal directions.

Conventions.

The colour as used by the author is encoded. In foreign literature the English equivalent of the colours has been used.

8. Relation COLOUR.

COLOUR (REF.NO. , COLOUR)

The colour of the mineral in reflected light.

Convention.

As 7.2.

9. Relation CHEMISTRY.

CHEMISTRY (REF.NO. , OXIDE , VALUE).

Contains the major elements of a chemical analysis.

9.1. OXIDE.

The oxide name is encoded in the form used by the author. This may include somewhat unusual oxidation states of multivalent atoms for example Ti_2O_3. Terms such as SUM, TOTAL or O=F, O=CL are also included.

9.2. VALUE.

The value, in weight per cent, of the major element.

Conventions.

The number of deimal places in the original analysis has been retained as an indication of the accuracy of the analysis. Detection limits given in the form>0.01, < 0.01 etc. have been encoded as the number itself e.g. 0.01. Non-numeric responses such as 'n.det', 'n.d.', 'tr' have all been ignored and no response entered.

10. Relation TRACE.

TRACE (REF.NO. , ELEMENT , VALUE)

Consists of the name and value for the trace elements. A trace element is distinguished from a major element only in having ppm as units of measurement.

10.1 ELEMENT.

The name of the element.

10.2 VALUE.

The amount in ppm of the trace element present.

11. Relation TECHNIQUE.

TECHNIQUE (REF.NO. , EXAMINATION , ANALYTICAL-METHOD)

Contains information concerning the experimental techniques used to investigate the specimen plus other useful notes concerning contaminants etc.

11.1. EXAMINATION.

Experimental techniques which have been applied to the specimen but the results of which would not enter the data file anywhere else.

Conventions.

A number of standard responses have been entered for this field, these include 'X-RAY', 'INFRARED', 'MOSSBAUER', the latter two

have been abbreviated to 'IR'. and 'MOSS'. for those specimens for which more than one technique is recorded. X-RAY implies a site population study. D.T.A. is used as the abbreviation for Differential Thermal Analysis.

11.2. ANALYTICAL-METHOD.

The analytical technique as applied to the specimen, plus any useful notes are included here.

12. Relation PHYSICAL.

PHYSICAL (REF.NO. , PROPERTY , VALUE)

Contains the physical properties, Specific Gravity, Density, and Hardness.

12.1. PROPERTY.

The name of the physical property.

Conventions.

The conventional form of the properties are 'S.G.' for specific gravity, and 'HARDNESS' and 'DENSITY'.

10.2. VALUE.

The value taken by the physical property.

Conventions.

Only the observed, not the calculated, value for the specific gravity or density have been encoded. The number of decimal places as used in the original source has been maintained as an indication of accuracy. Where a range of values for the hardness existed the mean value has been entered.

13. Relation STRUCTURE.

STRUCTURE (REF.NO. , CELL PARAMETER, VALUE, ERROR)

Contains information relevant to the unit cell. The space group of the unit cell, where given, is to be found in relation

SYMMETRY.

13.1. CELLPARAMETER.

Name of the unit cell parameters e.g. A, B, C, BETA, VOLUME.

13.2. VALUE The numerical value for the cell parameters.

Conventions.

The authors number of decimal places is retained as an indication of accuracy. Angles are quoted only in decimal degrees. The value for the beta angle has been taken directly from the original source. At times beta has been used for both the acute and obtuse angle.

13.3. ERROR.

The explicitly described error in determining the cell parameter.

Conventions.

See 6.2.

14. Relation SYMMETRY.

SYMMETRY (REF.NO. , SYMMETRY).

Describes the space group symmetry if this explicitly given.

15. Relation COEXISTENCE.

COEXISTENCE (REF.NO. , OTHER-REF. NO.)

A cross-linkage between two, or more, specimens which either coexist or show exsolution relationships.

Conventions.

Before the linkage is made there must exist definite evidence that either of the above conditions hold. A description of two specimens by different authors from the same 'locality' is not

taken as sufficient evidence of coexistence. The entry is in the form of the two reference numbers with the numbers alternatively in each domain, thus if specimens 4567,7896 coexisted two tuples would be entered containing respectively 4567,7896 and 7896,4567.

16. Relation EXTRA.

EXTRA (REF.NO. , OTHER-REF.NO.)

A cross-linkage between two, or more, separate pieces of information published from different 'references' relating to the same amphibole specimen.

Conventions.

Description of material collected from the same locality and assumed to represent identical material as used in some previous investigation has been excluded. The relation is constructed as COEXISTENCE.

17. Relation REDETERMINATION.

REDETERMINATION (REF.NO. , OTHER-REF. NO.)

A crosslinkage between two, or more, analyses of the same specimen by the same or different authors.

Conventions.

The relation is constructed as COEXISTENCE.

DURHAM UNIVERSITY
27 OCT 1976